Succession in plankton communities
A trait-based perspective
The research presented in this thesis was carried out at the Department of Theoretical Biology, Vrije Universiteit Amsterdam, The Netherlands.

**Cover picture:** This thesis proposes to model all species in the ecosystem with one single, *general purpose* model. Species differ only in the amount of energy they invest in each of their different activities (the tools of the Swiss army knife), not in the rules that specify their behaviour.

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Succession in plankton communities
A trait-based perspective

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Summary

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1 General introduction

1.1 Context

1.1.1 The biological carbon pump

Marine ecosystems exert a direct influence on the global climate. Strikingly, this influence is primarily attributed to the smallest organisms (0.2 – 200 µm) living in our oceans: the phytoplankton. Although this group of organisms constitutes only 0.2 % of the total photosynthetic biomass on earth, it is responsible for up to 50 % of the global primary production (Falkowski and Raven 2007; Field et al. 1998).

How it works

In the well-illuminated surface layer of the ocean (the top 100-200 m) phytoplankton produces new biomass from CO$_2$, which is continuously replenished from the atmosphere. Newly produced biomass enters the marine food web, feeding herbivores such as zooplankton, which in turn support higher trophic levels including fish. Most of the produced biomass is ultimately recycled near the surface, returning to inorganic nutrients that again fuel (secondary) production. However, a few percent sinks into the deep ocean as “marine snow”. Thus, the initial action by phytoplankton has effectively transported CO$_2$ from the atmosphere to the deep ocean. This process is referred to as the biological carbon pump (Volk and Hoffert 1985).

Long term effect

The bulk of the organic carbon that reaches the deep ocean is ultimately remineralized by microbial activity. This locally elevates the concentration of CO$_2$ and other inorganic nutrients, which then slowly find their way back to the surface through diffusion. If the sinking continuous for a sufficiently long time, deep water CO$_2$ will build up until upward diffusion of carbon completely balances the sinking. At that point, a steady-state has been reached: no net carbon transport occurs at any depth, and the uptake of CO$_2$ across the ocean surface is zero. Intriguingly, the sinking-mediated export of CO$_2$ therefore does not necessarily translate into a net flux of CO$_2$ into the ocean. Rather, it establishes a partitioning between the surface (surface ocean and atmosphere) and deep ocean, with the deep harbouring a higher concentration of CO$_2$. This demonstrates the analogy between the biological carbon pump and the cellular ion pumps for which it was named: a continuous, active transport mechanism serves to maintain a concentration gradient. It is estimated that this balance between sinking and upward diffusion existed over the 10,000 years preceding the industrial revolution (Raven and Falkowski 1999).

Future perspectives

It has been calculated that the biological pump causes the deep ocean to hold about 150 µmol kg$^{-1}$ more inorganic carbon than the 2120 µmol kg$^{-1}$ that would be expected...
1. General introduction

from the known surface concentration and physical processes alone (Raven and Falkowski 1999). This suggests that the atmospheric CO\textsubscript{2} concentration would be significantly higher in the absence of the biological pump. However, the present role of the biological pump does not offer guarantees for the future. Due to anthropogenic emissions, the concentration of CO\textsubscript{2} in the atmosphere continues to rise. This will affect the marine environment: temperatures will increase and the mixing intensity and pH will decrease. Each of these factors is of significant importance for ecosystems, both for bulk properties such as the elemental composition and export of organic matter (Laws et al. 2000; Riebesell et al. 2007) as for the species composition (Falkowski and Oliver 2007; Orr et al. 2005). However, the net effect of this pallet of changes on the biological pump is uncertain, and requires a thorough understanding of the processes at play.

1.1.2 Why the ecosystem matters

Long term control: the role of stoichiometry

The steady-state balance between sinking organic matter and upward diffusion of inorganic matter applies not only to carbon (C), but also to other nutrients such as nitrogen (N) and phosphorus (P). If the upward and downward transports operate indiscriminately on all nutrients, the diffusion-driving vertical gradients in the different inorganic nutrients must be proportional to each other, which proportionality constants equal to the corresponding stoichiometric ratios (C:N:P) in the sinking organic matter. The mean stoichiometry (i.e., elemental composition) of marine organic matter is remarkably well conserved, as was first noted by Redfield (1934): carbon, nitrogen, and phosphorus tend to occur in the so-called Redfield ratio of 106:16:1. If the stoichiometry of organic matter is constant in depth, the proportionality between vertical gradients of different nutrients translates in a similar proportionality between the surface-deep concentration differences for these nutrients. If nutrients (nitrogen or phosphorus) are depleted at the surface, this renders a remarkably simple relationship: the difference in CO\textsubscript{2} concentration between the surface and deep ocean is equal to the deep water nutrient concentration, multiplied by the carbon-to-nutrient ratio in sinking organic matter (Omta 2009; Redfield 1958). The long-term contribution of the biological pump thus hinges on two parameters: the deep water concentration of the limiting nutrient, and the corresponding carbon-to-nutrient ratio in organic matter.

The steady-state analysis suggests that the sole aspect of the biological pump that is under direct biological control, is the carbon-to-nutrient ratio in sinking organic matter. Therefore, the future, long-term behaviour of the biological pump depends on the changes in the stoichiometry of organic matter, under the influence of increased atmospheric CO\textsubscript{2} and associated global warming. This led Omta et al. (in press; 2006) to study the dependence of the stoichiometry of a single algal population on light intensity (mediated by mixing depth) and temperature.
Species composition

It is doubtful whether developments in the stoichiometry of sinking organic matter can be inferred from the properties of a single population of algae. The final composition of sinking matter is a result of the complex interplay of different members of the ecosystem, with phytoplankton species varying substantially in stoichiometry, and zooplankton and bacteria selectively incorporating and exudating the different constituents of their substrate based on stoichiometry. Moreover, the composition of sinking organic matter does not necessarily mirror that of the living ecosystem, as only certain types of organic matter (e.g., large diatoms, faecal pellets, polysaccharide-rich aggregates) have non-negligible sinking rates. As a result, it is difficult to make reliable predictions on the future stoichiometry of sinking matter without information on the structure of the ecosystem, and the interaction of its members (Thingstad et al. 2008). Such details become even more relevant when we consider the transient, shorter time scales over which the ocean will adjust to increased levels of atmospheric CO$_2$. This rate of adjustment relates to the sinking rate of organic matter, which is highly sensitive to particle size and density (Jackson and Burd 1998; Kriest and Oschlies 2008) – in turn strongly influenced by the composition of the phytoplankton community and the presence of predators. Robust estimation of the working of the biological pump necessitates a representation of the marine ecosystem that is at least sufficiently detailed to resolve variation in stoichiometry and sinking rate.

Ecosystem flexibility

Marine ecosystems are highly flexible: their structure varies in time and space. Temperate plankton communities undergo pronounced seasonal succession, with spring communities of sinking diatoms being consumed by rapidly increasing populations of zooplankton, then to be replaced by motile mixotrophic flagellates over the course of summer. Similarly, the structure of the marine ecosystem varies substantially with geographic location: high-production, high-export systems can be found at high latitudes, whereas low-biomass, oligotrophic systems are found near the subtropics and tropics. It would be a fallacy to expect present-day ecosystems to be unaffected by climate change: it is believed that changes in temperature, pH and mixing intensity already induce shifts in the species composition of ecosystems (Briand et al. 2004; Nehring 1998; Occhipinti-Ambrogi 2007). That suggests that a throughout analysis of the biological carbon pump must resolve the principles that govern changes in species composition under the influence of environmental change.

1.2 Marine ecosystem models

A quantitative assessment of the biological pump requires models that formalize our knowledge of the different mechanisms at play in terms of mathematical equations. These models can then be used to assess the status quo, and to produce forecasts and hindcasts for the behaviour of marine ecosystems and the biological carbon pump.
1.2.1 Prior work

Pioneers in marine ecosystem modelling reproduced key features of real plankton communities by stacking simple process-based descriptions of a few trophic levels. This resulted in the well-known nutrient-phytoplankton-zooplankton (NPZ, Evans 1988) and nutrient-phytoplankton-zooplankton-detritus (NPZD, Fasham et al. 1990) models. These succeed in reproducing several characteristic features of marine systems, such as the timing of the spring phytoplankton bloom. However, in their aim for a canonical description of the marine ecosystem, they unavoidably limit the representation of the species composition of the community. This makes these models rather unsuitable for the quantification of the biological pump, which subtly depends on the structure of the ecosystem.

Over the past two decades, the same modelling philosophy of “stacking trophic levels” was adopted to construct more complex plankton functional type (PFT) models (Baretta et al. 1995; Quéré et al. 2005). These allocate a separate variable to each group of species that is thought to fulfil a distinct role in nature, and they could potentially go down to the level of individual species if warranted by their unique ecosystem function. PFT models have an obvious appeal, as they directly mirror the diversity and species composition of actual marine systems. However, they also suffer from problems: the presently available laboratory and field observations cannot constrain many of the model parameters. There is simply not sufficient information available on the processes and organisms modelled. Since some of the modelled species are difficult or impossible to culture, the information needed to constrain such complex models may never be obtained. This led Anderson (2005) to question whether incorporating such levels of detail in ecosystem models is a feasible approach. This quickly became the topic of hot debate (Anderson 2006; Flynn 2006; Quéré et al. 2005).

1.2.2 Constructing an alternative

The traditional approach to ecosystem modelling quickly reaches its limits if there is a need to resolve species composition and diversity – at some point existing empirical knowledge does not suffice to parameterize the increasingly complex models. This is easily recognized. However, alternative approaches are not readily available: it is seemingly impossible to mathematically describe the detailed behaviour of a natural system without exhaustive information on the underlying mechanisms. Yet this is precisely what the present study aims for: by combining general principles that govern interspecific variation with a model of the community as a single adapting entity, an attempt is made to describe the marine ecosystem with a minimal model that preserves key elements of natural diversity.

From evolutionary Adaptive Dynamics to species succession

Inspiration for this work comes from the Adaptive Dynamics (AD) approach to the modelling of evolution (Dieckmann and Law 1996; Metz et al. 1996; Troost 2006), which was recently applied to a variety of questions in aquatic ecology (Jiang et al.
1.2 Marine ecosystem models

2005; Litchman et al. 2009; Troost et al. 2008; Troost et al. 2005a; Verdy et al. 2009). AD describes evolution as the replacement of a resident species by an invading mutant, in an environment that is completely determined by the resident. Reproduction of the resident creates mutants, which differ only very slightly and randomly in the value of continuously valued traits. For the sake of simplicity most models allow only a subset (typically one or two) of all organismal traits to evolve; a typical example is the asymptotic size of the species. A mutant invades and replaces the resident only if the mutant traits are competitively superior. Thus, the direction of selection naturally emerges as a result of competition between resident and mutant.

While species physiology and behaviour do influence the outcome of evolution, both the direction and rate of evolution tend to be dominated by the cost and benefit associated with a change in trait value. Thus, the pivotal step is the definition of trade-offs associated with the traits of interest. For the trait body size, for instance, such trade-offs often incorporate body size scaling relationships that connect a wealth of physiological characteristics to the size of the individual organism (Kooijman 2000; Troost et al. 2008). In a sense, AD can be considered to let the evolution of an ecosystem emerge from a few simple building blocks: trade-offs, random variability, and competition.

AD specifically targets evolutionary processes and makes assumptions accordingly. Notably, it is assumed that all variability stems from mutation, and that ecological processes operate on much shorter time scales than evolution. The latter implies that the ecosystem contains only the resident and is in equilibrium when a new mutant is introduced. It would be intriguing, however, if these assumptions could be relaxed: by allowing introduction of mutants and selection to occur at the same time – allowing coexistence of multiple types – and introducing other sources of trait value variability (e.g., immigration), the framework comes to describe succession in ecosystems, including their adaptive response to spatiotemporal environmental variability. This idea underlies several studies that consider "adaptive dynamics" (note the lack of capitalization) of communities on ecological time scales (Abrams et al. 1993; Norberg et al. 2001; Savage et al. 2007; Wirtz and Eckhardt 1996). This thesis incorporates and extends this concept: the marine ecosystem is allowed to self-assemble from an large assemblage of species, differing only in the value of one or two traits, subject to trade-offs.

The adapting ecosystem and the role of spatiotemporal heterogeneity

When translated to ecological time scales, the principles of Adaptive Dynamics bear a strong resemblance to Complex Adaptive Systems (CAS) theory (Holland 1996; Levin 1998). Though this is primarily a conceptual framework without direct implications for modelling, it is useful in that it identifies three ingredients that allow the ecosystem to behave as a distinct adapting entity: (1) sustained diversity and individuality of system components, (2) localized interactions between components, and (3) an autonomous process that selects components based on the outcome of the
interactions. Most of these elements can be recognized in Adaptive Dynamics: sustained diversity is guaranteed by mutation (immigration on ecological time scales), individuality by the variation in trait value, and an autonomous selection process is provided by competition.

The CAS requirement of localized interaction merits closer observation. It typically refers to localization in time- and/or space: by allowing the environment to vary, the optimal trait value can become a moving target that is never attained. A certain level of localization is implicit in the time scale separation employed by Adaptive Dynamics: competition between a new mutant and the resident is allowed to take its course before any new types are introduced. When ecological and evolutionary time scales come to overlap, however, this separation is no longer guaranteed. Without other means of localizing interactions, this all-to-easily results in competitive exclusion (Hardin 1960), in which a single optimal species thrives at the expense of all others.

In aquatic systems, localization of interactions exists on multiple fronts. Seasonal and inter-annual variation guarantee a dynamic environment, particularly in temperate regions. This can be accounted for in models by imposing temporal variation in temperature, light and other environmental variables. Spatial variability plays an important role as well: there exists strong variability in depth and latitude of environmental variables such as light, nutrient concentration and temperature. As the mixing between these different regions is limited, this variation ensures the persistence of ecologically different patches with slow migration between them. This can be modelled implicitly with metacommunities (Leibold and Norberg 2004) or explicitly with hydrodynamic models in which biotic and abiotic variables are transported through advection and diffusion. The potential of the latter is illustrated in the study by Follows et al. (2007), whose self-assembling ecosystem embedded in a hydrodynamic model of the world ocean successfully reproduces key aspects of natural marine systems.

The General Ocean Turbulence Model

Because of the defining role of environmental variability for natural plankton communities, this thesis pays significant attention to the detailed resolution of spatial and temporal variability of the aquatic environment. This is achieved by embedding the plankton community models in the General Ocean Turbulence Model (GOTM): a detailed one-dimensional hydrodynamic model of the marine water column (Burchard et al. 2006; Burchard et al. 1999). This model focuses on resolving the time- and depth-varying turbulent mixing, which controls the distribution of nutrients and biota over the water column. Near the surface, the mixing is primarily controlled by atmospheric variables, such as the wind speed and air temperature. In this thesis, the values for these variables are derived from observed meteorological conditions, which implies that seasonal, diurnal and other (chaotic) variability at the surface are all accounted for. Through the turbulence module, this temporal variation is translated into a temporally and spatially varying mixing intensity. This resolves
characteristic patterns in mixing intensity, such as the cold- and wind-driven deep winter mixing (which introduces nutrients from the deep) and summer stratification. Additional spatial variability is created through the decay of the light intensity with depth. Combined, these model components result in an aquatic environment that varies realistically in both time and space.

The GOTM permits the embedding of custom biotic and abiotic tracers, which are then transported accordingly through advection and (turbulent) diffusion. A key main benefit of this direct embedding is that it allows direct application of the GOTM library of numerical schemes for advection, diffusion and time integration to the biological models. This takes away the need of implementing such schemes from scratch, which would not be a trivial task. Nevertheless, as part of the present study several new time integration schemes have been developed and integrated in the GOTM (Broekhuizen et al. 2008; Bruggeman et al. 2007).

**Dynamic Energy Budget theory**

Self-assembly of ecosystems is no magical solution to all problems in ecosystem modelling. Lessons learned from community assembly studies (Drake 1990; May 1974; Morton et al. 1996; Post and Pimm 1983) indicate that the results of self-assembly are highly sensitive to the precise implementation of the assembly process and to the chosen interspecific differences. The latter implies that in a trait-based approach, the outcome of competition will depend strongly on the selection of traits and on the specific trade-offs imposed.

To make well-informed decisions in these matters, all models, trait and trade-offs are based upon concepts from Dynamic Energy Budget (DEB) theory (Kooijman 2000). DEB theory presents a concise, unified modelling framework for describing the quantitative behaviour of individual organisms. It easily accommodates lower levels of organization (biochemical pathways) as well as higher levels (populations). The DEB framework has been successfully applied to a large variety of organisms, literally ranging from bacteria to whales. Moreover, it is demonstrably capable of bridging traditionally different domains with a single model: a DEB-based mixotroph smoothly varies between generalized mixotrophy and specialized autotrophy and heterotrophy, depending on the environment. (Kooijman et al. 2002; Troost et al. 2005a; Troost et al. 2005b). This provides an ideal basis for the modelling of adapting communities, which will shift strategies depending on their environment.

DEB theory emphasizes the mechanisms that underlie the behaviour of natural systems. In many of these mechanisms trade-offs are already implicit. For instance, the DEB model introduces a straightforward partitioning rule to describe the allocation of energy to reproduction and other metabolic activities. The corresponding allocation coefficient is by definition subject to a trade-off: allocating more energy to reproduction comes at the expense of growth. Such partitioning principles are used extensively in this thesis to obtain trade-offs.
1. General introduction

**Aggregation**

Modelling the self-assemblage of an ecosystem through competition requires the simultaneous simulation of many different species, which is computationally expensive. A key attraction of Adaptive Dynamics is that it provides a concise mathematical description of the expected trait dynamics throughout evolution. Rather than tediously having to simulate the emergence of individual mutants and their competition with the resident, it is under certain circumstances possible to directly describe the expected evolutionary change in trait value with the "canonical equation" (Dieckmann and Law 1996). This equation depends only on the reproduction rate of the resident, the mutation rate and variance, and – critically – the trade-off associated with the traits undergoing evolution.

However, the AD canonical equation is built directly upon the assumption of separated ecological and evolutionary time scales, specifically by assuming that the standing diversity is always zero (only the resident is present) and that trait value variability stems from mutation only. Fortunately, it is possible to derive very similar equations for the case when ecological and evolutionary time scales meet (Norberg et al. 2001; Savage et al. 2007; Wirtz and Eckhardt 1996). As these equations describe a more general problem, they lack the certainty of the AD canonical equation; by design, they approximate the actual dynamics of the system. In doing so, they reduce a full model with potentially hundreds of species to a limited number of community statistics. In doing so, they greatly decrease the computational cost associated with running these models, at the cost of slightly reducing the accuracy of the model predictions.

**Aims**

In short, the present study aims to reproduce the behaviour of marine ecosystems, particularly plankton communities, in a detailed spatially and temporally varying environment. The ecosystem is allowed to self-organize though competition among large collections of virtual species. These species differ in the value of one or more traits, subject to trade-offs, and are modelled according to principles from DEB theory. Approximations for the dynamic behaviour of a few key community statistics are then introduced to obtain a computationally efficient approach. This enables the study of self-assembling communities in detailed one-dimensional and three-dimensional hydrodynamic models. Together, these components provide a complete modelling framework for the study the role of species composition and diversity in the marine ecosystem. This can directly aid climate studies that aim to resolve the present and future behaviour of the biological carbon pump.

**1.3 Outline**

Chapter 2 emphasizes the role of community diversity (as opposed to physiology) in determining key features of the marine ecosystem. This idea is developed with a model of a self-assembling phytoplankton community with two traits: the investment in light harvesting and the investment in nutrient harvesting. The assemblage of
species is modelled explicitly: both trait axes are discretized to produce a collection of several hundreds of species. These compete within a one-dimensional model of the marine water column, in which biota are transported by turbulent diffusion. The water column is subjected to realistic temporally varying forcing. Spatial and temporal patterns that emerge from this model are shown to agree well with classic observations in natural systems.

Chapter 3 describes in detail how the behaviour of large assemblages of species may be approximated with a few variables: the total community biomass, the mean of the traits (a measure of community strategy), and the covariances of these traits (a measure of functional diversity). This work builds directly upon previous studies, but extends these to multiple traits, log-normal trait distributions and discusses transformations that may be used to integrate these variables in advection-diffusion models.

Chapter 4 applies the newly developed aggregation method to a mixotrophic plankton community with traits representing the investments in autotrophy and heterotrophy. Again, this model is embedded in a one-dimensional model of the water column. Comparison with an explicitly modelled assemblage of species indicates that the approximate aggregation method performs well, in particular in predicting biomass and community strategy. Furthermore, the model displays patterns in community strategy (autotrophy, mixotrophy and heterotrophy as function of time and depth) and diversity that agree remarkably well with a large variety of observations on natural systems.

Chapter 2 and 4 already illustrate the difficulty of selecting traits and trade-offs: the capacities for light harvesting, nutrient harvesting and mixotrophy all mediate phytoplankton growth, as do many other unexplored traits (e.g., size, susceptibility to predation). However, the number of traits that can realistically be incorporated in a model is limited, as each addition trait requires additional information on associated trade-offs. As the choice of traits and trade-offs largely determines the outcome of the competition within species assemblages, it is of key importance that these deliver the best possible representation of the variability among natural species. The remaining chapters are, therefore, dedicated to the identification of dominant traits and trade-offs.

Chapter 5 presents a generic method for connecting trait value observations across species with a unified evolutionary model. This canonical model is based on the concept of genetic drift, and operates directly on a set of observations and the species phylogeny. Application of the model to a set of observations renders several useful results. First, this allows reconstruction of approximate trade-offs that govern evolutionary change. These trade-offs can be used as basis for adaptive models such as presented in chapter 2 and 4. Second, recombination of these trade-offs with the original observations and phylogeny allows the model to predict trait values for all taxa. This works even if no direct observations on the taxon are available.
Chapter 6 demonstrates the potential of the evolution-based model by applying it to a database with observed values for phytoplankton traits. This newly constructed database contains over one thousand observations on the size, growth rate, nutrient affinity, and susceptibility to predation of freshwater phytoplankton species. These observations are combined with a qualitative phytoplankton phylogeny to produce estimates for the traits of a wide range of phytoplankton taxa. The usefulness of these predictions goes beyond the models presented in this thesis: they can contribute to any modelling effort involving phytoplankton.

Summarizing, this study presents a conceptual, trait-based approach that views marine plankton communities as single adapting entities. This concept is developed in a mathematical framework for the efficient modelling of such communities, tailored to work well in hydrodynamic models. In addition, ideas are presented on how the abstract concept of traits and trade-offs may be related to real-world observations. Specifically, a method is presented that unifies scattered observations across taxa with a model that explicitly considers phylogenetic relationships; this model can then directly be used to identify dominant traits and trade-offs.

1.4 References


1. General introduction


1. General introduction
2 A biodiversity-inspired approach to aquatic ecosystem modeling


Abstract
Current aquatic ecosystem models accommodate increasing amounts of physiological detail, but marginalize the role of biodiversity by aggregating multitudes of different species. We propose that at present, understanding of aquatic ecosystems is likely to benefit more from improved descriptions of biodiversity and succession than from incorporation of more realistic physiology. To illustrate how biodiversity can be accounted for, we define the System of Infinite Diversity (SID), which characterizes ecosystems in the spirit of Complex Adaptive Systems theory as single units adapting to environmental pressure. The SID describes an ecosystem with one generic population model and continuity in species-characterizing parameters, and acquires rich dynamics by modelling succession as evolution of the parameter value distribution. This is illustrated by a 4-parameter phytoplankton model that minimizes physiological detail, but includes a sophisticated representation of community diversity and interspecific differences. This model captures several well-known aquatic ecosystem features, including formation of a deep chlorophyll maximum and Margalef-like nutrient-driven seasonal succession. As such, it integrates theories on changes in species composition in both time and space. We argue that despite a lack of physiological detail, SIDs may ultimately prove a valuable tool for further qualitative and quantitative understanding of ecosystems.
2. A biodiversity-inspired approach to aquatic ecosystem modeling

2.1 Introduction

Biodiversity poses a perennial problem for ecosystem modellers. Confronted with a reality fraught with species, dependencies and physiological detail, one cannot help but think that simple models cannot do it justice (Anderson 2005). Simple models aggregate large numbers of species into single state variables, and by doing so they lose the ability to reproduce ranges of behaviour shown by detailed species-explicit models (Raick et al. 2006). Also, the use of aggregation puts models at a greater distance from empirical results: First because assimilation of empirically-determined, species-specific parameter values to parameters of virtual aggregates of species is a difficult and largely subjective process; second because aggregate models provide only indirect information about individual species observed in the field. Not surprisingly, large ecosystem models that describe many classes of species explicitly have recently gained in popularity (Baretta et al. 1995; Quéré et al. 2005). However, continued diversification of functional groups may create more problems than it solves. Increasing the number of groups within ecosystem models dilutes the available empirical information per model unit, and therefore increases the uncertainty per parameter. Considering the substantial uncertainty already associated with parameters of moderate-size ecosystem models, this route seems unappealing. Also it is easy to overlook that as the number of variables within the ecosystem models increases, so does the amount on information needed to initialize the model: A utopian species-complete model would require initial abundances of every single ecosystem species (and their substrates) in order to arrive at accurate predictions. Even if it were possible, complete retrieval of this information is certain to prove so costly in practice that the actual value of such detailed models for most applications is debatable.

The merits of incorporating more species in ecosystem models are well recognized, but perpetually adding more explicitly modelled species primarily brings uncertainty and complexity. Instead, we propose a hybrid approach that builds on simple aggregate models, and bridges voids (in quantitative knowledge) between species classes according to unifying biological principles, e.g., thermodynamic constraints and body size scaling relationships. The use of a limited number of functional groups, in combination with interpolation based on unifying principles, replaces the unfeasible amount of species-specific information otherwise needed to model realistic diversity. To allow for interpolation between species, all species are modelled with the same, omnipotent population model; interspecific differences are captured by differences in values of key parameters – traits – rather than differences in model structure. Application of unified models to several similar species is not rare (Ebenhöh et al. 1997), but to our knowledge, such unification has not been applied consistently across ecosystems. Indeed, due to the large diversity within such systems, this is not a trivial affair: It places serious demands on the modularity and consistency of the model, and necessitates a modelling approach that spans species and functional groups. Such an approach is the Dynamic Energy Budget (DEB) theory (Kooijman 2000), which has been successful at describing a wide variety of species, and is
demonstrably capable of combining traditionally distinct strategies as autotrophy and heterotrophy (Kooijman et al. 2002; Troost et al. 2005a).

As next step toward simple biodiversity-based models, we assume continuity in trait values: Traits can take any value, and any combination of different trait values is possible in multi-trait models. In a sense, we allow for every conceivable hybrid between species. This concept offers a powerful means of system simplification, as illustrated by its application in earlier aquatic ecosystem models (Wirtz and Eckhardt 1996). Continuity in trait space implies that in a model that distinguishes n traits, the state of the system is described by an n-variable probability distribution, its value at any trait coordinate indicating the probability of finding a species with that specific trait value combination. Changes in ecosystem- and community structure are captured by the dynamics of the trait value distribution. We distinguish three mechanisms through which these dynamics arise: (1) succession, i.e., differential growth and decay of populations of the various species, (2) physiological adaptation, i.e., changes in the trait value of individuals (e.g., photoacclimation in the classic sense), and (3) genetic evolution, i.e., mutation and selection causing changes in the phenotype (trait values). Succession manifests as the rise of parts of the trait distribution at the expense of other parts, whereas physiological adaptation and evolution cause shifts in the distribution towards (local) fitness optima, on short and long time scales respectively. Each mechanism can be incorporated in trait distribution dynamics (Abrams et al. 1993; Dieckmann and Law 1996; Jiang et al. 2005); in this study we focus exclusively on succession. The resulting approach bears strong resemblance to Complex Adaptive Systems (CAS) theory (Leibold and Norberg 2004; Levin 1998; Norberg 2004), which aspires to understand (eco)system dynamics in terms of diversity and selection. Independent of the underlying mechanism, the direction and the rate of changes in the trait value distribution are in part governed by trade-offs associated with changes in trait value (Norberg 2004): The combination of (environment-dependent) costs and benefits of traits directs and bounds the evolution of the trait value distribution. Examples of trade-offs in aquatic systems abound: For phytoplankton, increased resource harvesting or defence against predation comes at the expense of growth (Wirtz and Eckhardt 1996), and harvesting of one nutrient comes at the expense of harvesting another (Huisman and Weissing 2001; Tilman et al. 1982).

Where the behaviour of traditional ecosystem models is for a significant part determined by parameter values, evolution of the trait value distribution depends on the shape of the initial distribution. If the system is opened to migration, this dependency is reduced as control shifts to the trait distribution of immigrating species. There are sound indications that in aquatic ecosystems migration can play a major role: “[we conceive] the pelagic as an open system where communities are continually reshaped by species immigration” (Cloern and Dufford 2005). With this in mind, we propose to model the ecosystem as a system that continuously experiences immigration of trace quantities of every possible species. Sources of immigrating individuals are not resolved explicitly, but may be found in (1) spatial subsidies (Polis et al. 1997), i.e., immigration from neighbouring environments as featured in
2. A biodiversity-inspired approach to aquatic ecosystem modeling

metapopulation theory (Hanski 1999; Leibold and Norberg 2004), or (2) permanent background concentrations of dormant life stages (e.g., spores, eggs) capable of awakening in viable environments (Anderson and Rengefors 2006). The rate of immigration may vary in time and place, and could – in particular when linked to spatial heterogeneity – correlate with water transports and/or (turbulent) diffusion. The fate of immigrating species is uncertain: The majority will perish (local extinction), but small subsets of species will at times find a niche, outcompete existing species and cause the trait distribution to change. The net result is reminiscent of a century-old concept from microbiology: "Everything is everywhere; the environment selects." (Baas-Becking 1934; Beijerinck 1913).

Summarizing, our approach encompasses three components: (1) an omnipotent population model, (2) trait distributions that capture biodiversity, and (3) continuous immigration of trace quantities of all species. We will refer to systems that incorporate these components as Systems of Infinite Diversity (SIDs). In this study, we demonstrate that a minimal, 4-parameter SID for phytoplankton, placed in detailed one-dimensional setting, reproduces a number of well-known aquatic ecosystem features, including: (1) seasonal development of a subsurface chlorophyll maximum independent of a biomass maximum (Fennel and Boss 2003) due to the emergence of a ‘shade flora’ (Sournia 1982b; Venrick 1982), (2) seasonal succession linked to variation in nutrient affinity, as proposed by Margalef’s Mandala (Margalef 1978), and (3) the suggestion of trade-offs between harvesting capacities for different resources in random samples of phytoplankton species (Huisman and Weissing 2001). The present incarnation of SIDs proves computationally expensive; in conclusion, however, we discuss recent techniques (Norberg et al. 2001; Wirtz and Eckhardt 1996) that are capable of rendering reasonably accurate, highly efficient parameterizations of SIDs.

2.2 Methods

In aquatic ecosystems, biodiversity has historically been extensively studied in terms of phytoplankton competition and succession (Margalef 1978; Sommer 1985; Tilman 1982); till this day, many ecosystem models still aim primarily to resolve and explain the rise and fall of phytoplankton species (Lancelot et al. 2005; Merico et al. 2004). Due to the substantial amount of data and theory available on phytoplankton succession, it presents an ideal test case for the SID approach. We therefore construct a simple model system that is limited to a phytoplankton community and one type of nutrient. The plankton model is loosely based on concepts from Dynamic Energy Budget theory (Kooijman 2000), and qualitatively resembles previous approaches (Diehl 2002; Huisman and Weissing 1995). Species interaction is implemented as competition for a shared external nutrient pool. The behaviour of the model is first evaluated in a non-spatial setting subject to a realistically fluctuating light intensity. Subsequently, we partially resolve the spatial structure of the environment with a water column model; this model incorporates a realistic time- and depth varying mixing intensity, and resolves the decrease in light intensity with depth.
2.2 Methods

2.2.1 A model of the phytoplankton community

Phytoplankton species differ quantitatively in numerous features, amongst which cell size, resource harvesting ability and edibility. In environments that are not predation-dominated (e.g., oligotrophic open ocean sites), a good predictor of the competitive ability of individual species is their affinity for nutrients and light (Passarge et al. 2006; Tilman 1982). To account for interspecific differences in nutrient- and light affinity, we propose to partition the total biomass of a phytoplankton population into three types: (1) biomass dedicated to light harvesting, (2) biomass dedicated to nutrient harvesting, and (3) structural biomass responsible for growth (cf. Geider et al. 1996; Klausmeier et al. 2004; Shuter 1979). Light harvesting biomass represents chlorophyll as well as closely associated cellular machinery. Similar to the work of Geider (1996; 1998) we assume a fixed fraction of light harvesting biomass to consist of chlorophyll, implying this type of biomass can serve as chlorophyll proxy. Nutrient harvesting biomass includes compounds directly affecting nutrient consumption (e.g., membrane-bound transporters), as well as any co-occurring machinery. If one accepts that the capacity for nutrient uptake is determined by the surface area of the cell (Munk and Riley 1952; Sournia 1982a), nutrient harvesting biomass must comprise the "shell" of the cell, i.e., the cell wall and membrane as well as transporters. Then the ratio of nutrient harvesting biomass to structural biomass can serve as proxy for the surface-to-volume ratio, and for isomorphic species its reciprocal can be a proxy for cell size (Kooijman 2000). However, this relationship is obfuscated if diffusion limits nutrient availability (Chisholm 1992), as may occur in oligotrophic environments; we
therefore do not explore the link between nutrient harvesting biomass and size further in this study. Structural biomass represents all biomass that does not contribute to assimilation, but is required to build a living alga; it can be regarded as a measure of population size. In the model we quantify the species-specific distribution of biomass over the three pools by two partition coefficients: $m_L$ represents the quantity of light harvesting biomass per unit of structural biomass, and $m_N$ represents the quantity of nutrient harvesting biomass per unit of structural biomass. One can interpret these coefficients as harvesting investments: They quantify a species’ investment in resource harvesting, relative to its investment in pure growth. The combination of the partition coefficients and the amount of structural biomass, denoted by $g_{1848}$, specifies the amount of light- and nutrient harvesting biomass:

$$g_{1865} \frac{m_L}{g_{3013}} + g_{1865} \frac{m_N}{g_{3015}}$$

A phytoplankton population is assumed to require light and some nutrient (e.g., nitrate) to produce new biomass. The rate of biomass production is governed by the synthesizing unit (SU) expression for colimitation, which offers a flux-based description of classic multi-substrate enzyme kinetics under the assumption of negligible substrate dissociation (Kooijman 1998; Kooijman 2000; Kuiper et al. 2004). The SU-governed rate at which new biomass is produced equals

$$J_A = \frac{1}{J_{Am}^{-1} + \left( \frac{J_L}{g_{1850}} \right)^{-1} + \left( \frac{J_N}{g_{1850}} \right)^{-1} - \left( \frac{J_L}{g_{1850}} + \frac{J_N}{g_{1850}} \right)^{-1}}$$

in which $J_{Am}$ denotes the maximum rate of biomass production, $J_L$ and $J_N$ the rates at which light and nutrient become available to growth machinery, and $g_{1850}$ and $g_{1850}$ the amounts of light and nutrient needed to produce one unit of biomass. The maximum rate of biomass production is taken proportional to the population size, quantified by the amount of structural biomass: $J_{Am} = r_{max}V$ with $r_{max}$ denoting the maximum structure-specific rate of biomass production. The internal availabilities of light and nutrient are taken proportional to the external light intensity $X_L$ and nutrient concentration $X_N$, respectively, and to the amounts of corresponding harvesting biomasses, i.e., $J_L \propto m_L V X_L$ and $J_N \propto m_N V X_N$. The rate at which new biomass is produced can now be written as

$$J_A = r_{max}V \frac{1}{1 + \left( \frac{m_L X_L}{K_L} \right)^{-1} + \left( \frac{m_N X_N}{K_N} \right)^{-1} - \left( \frac{m_L X_L}{K_L} + \frac{m_N X_N}{K_N} \right)^{-1}}$$

(2.1)

in which $K_L$ denotes the half-saturation light intensity at $m_L = 1$, and $K_N$ denotes the nutrient half-saturation concentration at $m_N = 1$. The half-saturation coefficients are compound parameters that contain yields $g_{18}$ and $g_{18}$ as well as the maximum growth rate $r_{max}$. Newly produced biomass is distributed over the three biomass pools as
specified by the partition coefficients $m_L$ and $m_N$; thus, structural biomass is formed at rate

$$J_{VA} = \frac{J_A}{1 + m_L + m_N}$$  \hspace{1cm} (2.2)

We assume all biomass requires maintenance, i.e., a certain amount of energy per unit time necessary to maintain the cell (Kooijman 2000). Energy for maintenance is obtained through break-down of organic compounds; mass remineralized in this process re-enters the external nutrient pool. As initial approximation, we will assume that all three biomass types are subject to equal maintenance requirements. Additionally, we assume that only structural biomass can serve as energy source for maintenance; energy stored in harvesting biomasses (e.g., chlorophyll) cannot be regained. Harvesting biomasses simply decay passively along with structural biomass. The rate of structural biomass turnover related to maintenance is now given by

$$J_{VM} = (1 + m_L + m_N)k,$$  \hspace{1cm} (2.3)

in which $k$ denotes the amount of structural biomass required to maintain one unit of (structural or harvesting) biomass per unit time.

The net growth of structural biomass equals the difference between assimilation and maintenance, i.e.

$$\frac{dV}{dt} = J_{VA} - J_{VM}$$  \hspace{1cm} (2.4)

Since the partition coefficients are constant for a given species, this immediately specifies the change in harvesting biomass: The dynamics of light harvesting and nutrient harvesting biomass equal $m_L \frac{dV}{dt}$ and $m_N \frac{dV}{dt}$, respectively. We choose to measure phytoplankton biomass in nutrient units (i.e., μmol nutrient L$^{-1}$), which implies that dynamics of the external nutrient pool mirror the dynamics of the total biomass: For a given change in structural biomass $\frac{dV}{dt}$, the corresponding change in nutrient equals $-\frac{dV}{dt}$.

The phytoplankton population model serves as basis of a System of Infinite Diversity (SID) in which all differences between phytoplankton species are quantified by differences in harvesting investments $m_L$ and $m_N$. These traits affect all parts of the metabolism: They enhance resource availability (Eq. (2.1)), but increase the cost for growth (Eq. (2.2)) and maintenance (Eq. (2.3)). This creates a trade-off between harvesting and net growth: If harvesting investments tend to zero, biomass growth stops while (structure-specific) turnover continues, resulting in extinction of the population. If harvesting investments become very high, assimilation saturates whereas (harvesting-specific) turnover increases linearly, also resulting in extinction. The trait values are thus restricted to a viable region, its environment-dependent contour defined by the trait value combinations for which $\frac{dV}{dt} = 0$. The largest
2. A biodiversity-inspired approach to aquatic ecosystem modeling

viable region is obtained if light- and nutrient availability are infinite; then we obtain the boundary

\[ m_L + m_N < -1 + \frac{r_{\text{max}}}{k}, \]

which in combination with the obvious boundaries \( m_L > 0 \) and \( m_N > 0 \) renders a triangular viable region: Species outside this region can never achieve a positive growth rate. Initial simulations show that of all species within the viable region, only a small fraction (< 20 %) with low trait values attains non-negligible biomass levels in practice. For all subsequent simulations, we therefore discretize the trait distribution for this smaller region only on a square 25 × 25 trait value grid; this renders a system composed of 625 virtual phytoplankton species. The dynamics of individual species are governed by Eq. (2.4), different for each species through the dependency on (species-specific) \( m_L \) and \( m_N \). All species share the external nutrient pool, the dynamics of which can therefore be written as sum of contributions of all species \( i \), i.e.,

\[
\frac{dX_N}{dt} = -\sum_i (1 + m_{L,i} + m_{N,i}) \left. \frac{dV}{dt} \right|_{v=v_i, m_L=m_{L,i}, m_N=m_{N,i}} \tag{2.5}
\]

2.2.2 Environmental conditions

The structure of phytoplankton communities is often strongly time- and space dependent. Seasonal fluctuations in solar radiation and mixing intensity drive succession, most prominently through the initialization of phytoplankton growth in spring (following stratification and increased solar radiation) and its termination in the fall (following increasing mixing and decreased radiation). Resource gradients in space – notably the exponential decrease of light intensity with depth – cause the community structure to be strongly space-dependent. Generally, one cannot separate the structure and diversity of communities from the heterogeneity of their environment: Biodiversity in nature is sustained at least partially because of spatiotemporal heterogeneity (Tilman 1982; Tilman and Kareiva 1997; Tilman et al. 1982). Therefore, we study the behaviour of the phytoplankton SID in a setting that includes variation in time and space. First, we simulate the phytoplankton community at an open ocean site over three years with a realistic time-varying light intensity, averaged over the top 150 m that constitutes the euphotic zone (Figure 2.2a). Second, we explicitly resolve the vertical structure of the top 400 m of the site with a 100-layer model of the turbulent water column (Burchard et al. 2006; Burchard et al. 1999); this model incorporates an exponential decay of light with depth, and calculates a time- and depth-varying mixing intensity (turbulent diffusivity) from observed weather conditions. The mixing regime controls the distribution of plankton and nutrient over the water column, and thus indirectly affects light- and nutrient availability. Figures 2.4a and 2.4b show the light intensity and turbulent diffusivity as function of time and depth. A detailed description of the water column model can be found in the appendix.
Table 2.1. Symbols used in the phytoplankton SID. Shown respectively: state- and forcing variables (the latter supplied by the physical model), traits, parameters, reference concentrations used for initialization and immigration, intermediate variables used in the model description only. Note that saturation coefficients $K_L$ and $K_N$ are references applicable when trait values $m_L$ and $m_N$ equal one, respectively; the effective half saturation coefficients equal $K_L/m_L$ and $K_N/m_N$.

<table>
<thead>
<tr>
<th>symbol</th>
<th>interpretation</th>
<th>unit</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V$</td>
<td>structural biomass</td>
<td>μmol L$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$X_N$</td>
<td>nutrient</td>
<td>μmol L$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$X_L$</td>
<td>light intensity</td>
<td>W m$^{-2}$</td>
<td></td>
</tr>
<tr>
<td>$D$</td>
<td>turbulent diffusivity</td>
<td>m$^2$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$m_L$</td>
<td>light harvesting investment</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>$m_N$</td>
<td>nutrient harvesting investment</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>$r_{max}$</td>
<td>maximum specific growth rate</td>
<td>d$^{-1}$</td>
<td>1.5</td>
</tr>
<tr>
<td>$K_L$</td>
<td>reference light half-saturation coefficient</td>
<td>W m$^{-2}$</td>
<td>2</td>
</tr>
<tr>
<td>$K_N$</td>
<td>reference nutrient half-saturation coefficient</td>
<td>μmol L$^{-1}$</td>
<td>0.25</td>
</tr>
<tr>
<td>$k$</td>
<td>rate of biomass turnover</td>
<td>d$^{-1}$</td>
<td>0.05</td>
</tr>
<tr>
<td>$κ$</td>
<td>immigration rate relative to turbulent diffusivity</td>
<td>m$^{-2}$</td>
<td>0.0001</td>
</tr>
<tr>
<td>$X_{N,ref}$</td>
<td>reference nutrient concentration for species $i$</td>
<td>μmol L$^{-1}$</td>
<td>4</td>
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<tr>
<td>$V_{i,ref}$</td>
<td>reference structural biomass concentration for species $i$</td>
<td>μmol L$^{-1}$</td>
<td>0.0008</td>
</tr>
<tr>
<td>$J_L$</td>
<td>light availability for biomass production</td>
<td>J L$^{-1}$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$J_N$</td>
<td>nutrient availability for biomass production</td>
<td>μmol L$^{-1}$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$y_L$</td>
<td>light needed per unit of produced biomass</td>
<td>J μmol$^{-1}$</td>
<td></td>
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<tr>
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<td>nutrient needed per unit of produced biomass</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>$J_{Am}$</td>
<td>maximum rate of biomass production</td>
<td>μmol L$^{-1}$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$J_A$</td>
<td>rate of biomass production</td>
<td>μmol L$^{-1}$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$J_{VA}$</td>
<td>rate of structural biomass production</td>
<td>μmol L$^{-1}$ d$^{-1}$</td>
<td></td>
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<tr>
<td>$J_{VM}$</td>
<td>structural biomass turnover due to maintenance</td>
<td>μmol L$^{-1}$ d$^{-1}$</td>
<td></td>
</tr>
</tbody>
</table>

### 2.2.3 Parameter values and initial conditions

Table 2.1 lists parameter values and the initial state used for the biological model. The water column is initialized with a nutrient concentration of 4 μmol L$^{-1}$, which is the average nitrate concentration across the top 400 m of the simulated open ocean site (Steinberg et al. 2001). An initial structural biomass concentration of 0.5 μmol L$^{-1}$ is distributed uniformly over the trait distribution grid, resulting in trace concentrations (0.8 nmol L$^{-1}$) of each of the 625 possible species. In both setups, we open the simulated nutrient-phytoplankton system by imposing a flow through the system. The flow introduces new nutrient and species at concentrations that are taken equal to the above initial levels, and simultaneously exports a fraction of the existing system. In the depth-averaged setup, the flow rate is constant (0.16 d$^{-1}$), whereas in the spatial setup

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this rate scales with the turbulent diffusivity, and therefore is time- and depth-dependent (typical flow rate: 0.00045 d\(^{-1}\) in summer to 2.6 d\(^{-1}\) in winter). Mathematically, the imposed flow is identical to dilution in a chemostat, diffusion between the modelled compartment and an outside source, or relaxation towards a reference state. Effectively, the flow reintroduces extinct species, and thus provides the permanent background diversity proposed for Systems of Infinite Diversity. Given its coupling with diffusivity, it is best thought of as a parameterization of horizontal transport and diffusion in a horizontally heterogeneous environment; its effect on diversity is similar to assumptions of a minimal population density (Burchard et al. 2006) or a constant diversity (Wirtz and Eckhardt 1996).

![Simulated light forcing](image1)

**Figure 2.2.** Simulated light forcing (a), nutrient and structural biomass (b), light harvesting investment (c) and nutrient harvesting investment (d) at the depth-averaged open ocean site. The light intensity is shown as the daily averaged signal (thin line) and its 90-day running mean (thick line). Structural biomass is integrated over the whole trait distribution, i.e., it equals the lump sum of all virtual species. Harvesting investments are shown as the non-normalized marginal densities of the bivariate trait distribution in time (gray scale), calculated by summing the discretized distribution (see also Figure 2.3) over one trait dimension and dividing by the grid step of the other trait. In addition it shows the means (solid line) and 10\(^{th}\) and 90\(^{th}\) percentiles (dashed lines) of the marginal densities.
2.3 Results

Figure 2.2 shows the light forcing and the response of biota- and nutrient levels at the depth-averaged open ocean site. The light intensity (Figure 2.2a) is visibly governed by a sinusoidal seasonal cycle on which noise due to rapid, erratic variation in cloud cover is imposed. Following the gradual increase in light intensity, a phytoplankton bloom begins in early spring (Figure 2.2b). In early summer most nutrient has been fixed in phytoplankton biomass. In the absence of grazers, this low-nutrient, high-biomass situation persists all over summer, to be finally terminated in autumn by the gradual reduction in light intensity. Figures 2.2c and 2.2d show the response of the phytoplankton community to changes in light and nutrient, visualized as the marginals (i.e., the individual distributions of light- and nutrient harvesting investments), means, and 10th and 90th percentile of the bivariate trait distribution over time. Foremost, one can observe that during the bloom, the typical light harvesting investment (e.g., its mean or modus) decreases slightly, whereas the nutrient harvesting investment increases. As species-specific harvesting investments are fixed, this indicates a change in community structure. Second, one can observe that the highest community diversity – quantified by the distance between the percentiles – occurs in winter; during the development of the bloom, diversity steadily decreases. Figure 2.3 shows the full bivariate trait distribution at the beginning (Figure 2.3a) and at the peak of the bloom (Figure 2.3b); again, the shift in investments and the decrease in diversity can be seen. We may note that Figures 2.2c and 2.2d are related to Figure 2.3: The former each show a marginal of the latter bivariate distribution – i.e., that distribution integrated over one trait axis – in time.
Figure 2.3. The discretized trait distribution at the start (a) and peak (b) of the bloom, at the depth-averaged open ocean site. Every bar represents a simulated virtual phytoplankton species; the height of the bar denotes the amount of structural biomass in that species.
2.3 Results

Figure 2.4. Simulated forcing, nutrient, biomass, and trait means as a function of time (horizontal) and depth (vertical) for the vertically-structured setup. Shown respectively: daily and 90-day running mean of the light intensity (a), turbulent diffusivity (b), nutrient concentration (c), structural biomass concentration (d), the mean light harvesting investment (e), and the mean nutrient harvesting investment (f). Structural biomass is integrated over the whole trait distribution, i.e., it represents the lump sum of all virtual species. Mean investments are masked where the total structural biomass does not exceed the immigrating background level of 0.5 μmol L⁻¹; this is the case in deep water, typically below 100 m. Gray scales correspond to the value of the plotted variables with white denoting complete absence, as indicated by the scale on the right. Only the top 200 m of the water column is shown; beyond this level, plotted variables do not change with increasing depth.
Resolution of the vertical structure of the site introduces several new phenomena: Light attenuation with depth produces a vertical gradient of light availability (Figure 2.4a), and a time- and depth-dependent mixing intensity (Figure 2.4b) controls distribution of nutrient and biomass over depth, as well as the rate of immigration. Despite these differences, the trends in nutrient (Figure 2.4c) and structural biomass (Figure 2.4d) in the upper layers resemble those seen for the depth-averaged setup: A phytoplankton bloom starts in spring, shortly after which the surface is depleted of nutrient; in autumn the community collapses and nearly all biomass is remineralized. Only beyond 100 m depth a different trend is seen: There, lack of light limits phytoplankton growth throughout the year and nutrient levels remain high. Similarly, the phytoplankton community structure in surface waters behaves qualitatively as in the depth-averaged setup: The mean nutrient harvesting investment increases while the bloom persists, at the expense of the mean light harvesting investment (Figures 2.4e and 2.4f). In deeper water (> 65 m), however, the mean light harvesting investment increases sharply at the onset of the bloom and remains relatively high throughout its lifespan, whereas the mean nutrient harvesting investment initially decreases to minimum levels and remains low. This switch between the nutrient- and light harvesting regimes occurs around 65 m, and could therefore not be reproduced with the depth-averaged setup, which described the top 150 m. Due to resolution of these two distinct regimes, the spatially explicit setup also permits more extreme trait value means: The effective ranges of mean light harvesting investments (0.17 – 0.62, Figure 2.4e) and nutrient harvesting investments (0.25 – 0.63, Figure 2.4f) are substantially larger than with the depth-averaged setup (respectively 0.39 – 0.56 and 0.47 – 0.53, Figures 2.2c and 2.2d).

2.4 Discussion

2.4.1 Phytoplankton community structure

The behaviour of the phytoplankton community can be viewed as a direct result of a time- and depth-varying environmental selection pressure. During the first few months phytoplankton experiences low light levels, due to low solar radiation as well as strong mixing (the latter in the vertically-structured setup only). In this period light limits phytoplankton growth to such extent that biota levels are nearly negligible and the nutrient concentration remains high. The few individuals that do persist are selected for light affinity rather than nutrient affinity; consequently, the column is at the onset of the bloom dominated by species with high investment in light harvesting (high $m_l$) and low investment in nutrient harvesting (low $m_n$). Shortly after the onset of the bloom, nutrient is depleted near the surface while light is amply available. This new situation favors species with high nutrient affinity, which can be seen to become more abundant as depletion persists. A different trend is seen in deeper waters (> 65 m) in the vertically-structured setup: There nutrient is more readily available as it diffuses upwards from nutrient-rich deep waters, whereas light intensity has dropped to such extent that it limits growth. This dark environment favours investment in light harvesting over nutrient harvesting, causing species with a high investment in light
harvesting (high $m_L$) to become more abundant. Species with high light affinity –
outcompeted by nutrient-harvesting species near the surface after the initial bloom
phase – thus manage to find a niche in deeper water layers. This summer situation is
reminiscent of the classic two-layer model with nutrient-limited dynamics near the
surface and light-limited dynamics near the deep (Dugdale 1967).

Figure 2.5. Light harvesting biomass as a function of time (horizontal) and depth (vertical) for the
vertically-structured setup. This quantity equals the product of structural biomass (Figure 2.4d) and the
mean light harvesting investment (Figure 2.4e), and can serve as chlorophyll proxy.

The product of the mean harvesting investment (Figures 2.4e and 2.4f) and the
structural biomass (Figure 2.4d) describes the biomass allocated to resource
harvesting, shown for light harvesting in Figure 2.5: Light harvesting biomass is high
at the onset of the bloom, and in deeper waters (85 m where 1.4 % of the surface
radiation remains) afterwards. It is common practice to assume that light harvesting
biomass consists in part of chlorophyll (Geider et al. 1996; Klausmeier et al. 2004).
Under this assumption, the model predicts formation of a maximum chlorophyll
concentration near the base of the euphotic zone, which persists independent of any
maximum in total biomass (which here – with neutrally-buoyant biota – is simply
highest near the surface; Figure 2.4d). This subsurface chlorophyll maximum is a well-
known, ubiquitous feature of aquatic ecosystems (Fennel and Boss 2003). Its
persistence independent of (structural) biomass has to our knowledge exclusively
been demonstrated in models that accommodate photoacclimation, i.e., regulation of
chlorophyll contents on the physiological level (Fennel and Boss 2003); this applies
for instance to the models of Geider et al. (1996; 1998). The present biodiversity-
inspired model demonstrates an alternative: A subsurface chlorophyll maximum can
arise through species sorting processes that favour high-chlorophyll 'shade' species in
the high-nutrient, low-light deep, as opposed to low-chlorophyll species with high
nutrient affinity near the surface. This matches the concept of a 'shade flora', i.e., the
idea that some species are preferentially located in deep levels of the euphotic zone,
which was put forward already at the end of the 19th century (Sournia 1982b). Variation in species assemblages with depth has been found at numerous locations including the simulated site (Biddigare et al. 1990; Kemp et al. 2000). Although the depth-specific assemblages of phytoplankton species are known to show great taxonomic variety (Sournia 1982b; Venrick 1982), they are commonly thought to show homogeneity in physiological features; early studies already suggested a link between preferential depth of species and their light affinity (Ryther 1956). It has been demonstrated that some deep-dwelling species are indeed capable of growing under very low-light conditions (Goldman 1993), indicating that these species indeed possess a higher light affinity. If we assume that light affinity correlates with chlorophyll content, these observations indicate that the subsurface chlorophyll maximum may indeed at least in part arise through local concentration of species with high light affinity and chlorophyll content, as suggested by our results.

In Margalef’s Mandala (Margalef 1978), phytoplankton succession is viewed as traversing a phase plane defined by nutrient concentration on the one hand and turbulence on the other: The initial high-turbulence, high-nutrient environment is replaced by a stratified depleted environment as the year progresses, with distinct niches for different groups of species (respectively: Diatoms, coccolithophorids, dinoflagellates) along this trajectory. Margalef explained this succession in terms of differential species-specific affinities for limiting nutrients, which in turn have been linked to morphology and cell size (Aksnes and Egge 1991; Chisholm 1992; Sournia 1982a). The concept of affinity-driven succession applies seamlessly to (near-surface) seasonal succession as observable in our results: As the bloom persists, colonizing species with low nutrient affinities are replaced by species with higher nutrient affinity. Thus, our result corroborates that nutrient availability and differences in nutrient affinity may control succession; this is also tentatively indicated by in-situ microcosm experiments demonstrating that nitrate addition in oligotrophic environments greatly changes the phytoplankton community structure (Carter et al. 2005).

Several studies have suggested that the capacities for light- and nutrient harvesting in phytoplankton might be negatively correlated (Huisman and Weissing 1995; Leibold 1997). In the present model such a correlation is not imposed: While the individual capacities for light- and nutrient harvesting are each independently governed by a harvesting-growth trade-off, the model does not incorporate an explicit negative feedback between light- and nutrient harvesting. Yet in Figures 2.4e and 2.4f a negative correlation between the two harvesting investments emerges: The environment appears to advocate either investment in light harvesting (in the dark) or investment in nutrient harvesting (in periods of depletion), but not both. Figure 2.6 illustrates that a slight negative correlation (~0.05) persists when integrating the trait distribution over time and space. As a result, random sampling of phytoplankton species could indicate a trade-off between light- and nutrient affinity. However, the indirect light-nutrient trade-off that emerges from our results is therefore not nearly as strong (in terms of correlation) as other phytoplankton trade-offs that have been
suggested to govern phytoplankton strategies (Huisman and Weissing 2001; Wirtz and Eckhardt 1996). If the mechanisms underlying our trade-off are real, its subtlety could explain why the existence of a trade-off between light- and nutrient harvesting has as yet not been convincingly demonstrated (Huisman and Weissing 2001; Passarge et al. 2006).

Figure 2.6. Depth- and time-integrated species abundance as function of light- and nutrient harvesting investment. The distribution is normalized so its integral equals one, and can consequently be interpreted as a probability distribution of combinations of harvesting investments. Note that harvesting investments \( m_L \) and \( m_N \) are inversely proportional to the effective half-saturation coefficients, which equal \( K_L/m_L \) and \( K_N/m_N \), respectively.

Not all differences in competitive ability between phytoplankton species relate to differences in light- and nutrient affinity. Some studies have argued against a determining role of nutrient affinity in seasonal succession (Smayda 1997; Smayda and Reynolds 2001), pointing out that nutrient affinity often is a poor predictor of the order of species appearance. For instance, diatoms commonly dominate the first, nutrient-rich stages of the spring bloom, but are known to possess high nutrient affinities. Smayda (1997) presented four alternative determinants of species appearance in the successional sequence: (1) nutrient retrieval mechanisms, (2) mixotrophic nutritional tendency, (3) allelochemically enhanced interspecific competition, and (4) allelopathic antipredation defence mechanisms. Of these mechanisms, the first can be accounted for in the present model: Nutrient harvesting biomass comprises all mass that directly or indirectly contributes to nutrient retrieval, and could therefore include structures that allow local motility, causing cells to shed stagnant water mantles that limit diffusion-mediated nutrient arrival. However, the other three mechanisms cannot directly be linked to nutrient harvesting biomass, and would therefore require qualitatively different models. Additionally, the current approach neglects direct selection by predators: If losses due to predation are
substantial, differences in phytoplankton fitness might better relate to the species’ susceptibility to predators than to differences in affinity (Carpenter and Kitchell 1996). The present study focuses primarily on succession in oligotrophic open ocean sites, where loss due to predation is often negligible (Steinberg et al. 2001); extension of the approach to aquatic environments where predation does play a role could necessitate the introduction of defence- or edibility traits (Wirtz and Eckhardt 1996). While beyond the scope of this study, we intend to investigate the role of other phytoplankton traits in the future. In particular mixotrophy is a suitable test case as it can be incorporated in SID type models through allocation rules (distinguishing autotrophic- and heterotrophic harvesting biomass), and would simultaneously allow the SID-approach to span more functional groups (e.g., heterotrophic bacteria) (Troost et al. 2005a); preliminary results indicate that differences in mixotrophic tendency can explain shifts in species composition and the ratio algae : bacteria in time and depth (in preparation).

2.4.2 Biodiversity

Changes in community structure are the result of selection pressure applied to assemblages of different species (Leibold and Norberg 2004; Levin 1998). The amount of diversity controls the rate at which the community responds to selection pressure (Norberg et al. 2001; Wirtz and Eckhardt 1996); diversity thus plays a major role in SID-type models that describe the adaptive behaviour of communities. The presence and persistence of biodiversity is often linked to spatiotemporal heterogeneity (Chesson 2000; Tilman and Kareiva 1997; Tilman et al. 1982). In the present study, temporal heterogeneity is established through a noisy seasonally fluctuating light intensity, which proves capable of inducing seasonal changes in community structure, independent of the presence of an explicit spatial structure (Figures 2.2c and 2.2d). However, the time-varying light intensity cannot sustain diversity: Similar to other studies (Norberg et al. 2001), most diversity is lost within a year if we do not impose continuous species immigration (not shown). For the vertically-explicit setup, one might expect spatial heterogeneity to sustain biodiversity. However, we find that the vertical light gradient combined with diffusion-mediated dispersal is insufficient for maintenance of a realistic biodiversity: In the absence of immigration from outside sources most diversity is again lost over time, though similar to other studies (Troost et al. 2005a) a low number of species appears able to coexist. Not surprisingly, the rate of immigration is a key parameter in both setups: A weak input cannot sustain substantial variance and causes the system to lose adaptive ability, whereas a strong input keeps the community close to its reference state and prevents it from adapting. In this respect, immigration as implemented in the vertically-structured setup arguably strikes an ideal balance: With immigration proportional to the turbulent mixing intensity, it nearly subsides in summer, allowing for significant specialization (i.e., changes in the mean trait value, Figures 2.4e and 2.4f), while in winter it greatly increases and resets the system to a state of high diversity. Consequently the system at times displays strong specialization without permanently surrendering a realistic level of diversity.
2.4.3 Systems of infinite diversity

A system of infinite diversity acquires rich dynamics through incorporation of competition and succession, and as such can display a wealth of realistic behaviours despite a lack of physiological detail and parameters. However, in their present form SIDs require considerable computational effort: discretization of the trait distribution requires many state variables to represent the different (virtual) species, which makes simulation expensive. This would discard the SID approach for many practical purposes, in particular for application in detailed spatially-explicit models such as General Circulation Models (GCMs). This problem can be avoided by abandoning discretization of trait distributions. Recent studies have shown that trait distributions are often well captured by the first distributional moments, i.e., mean, variance, skewness and kurtosis (Norberg et al. 2001; Wirtz and Eckhardt 1996). Rather than discretizing the distribution, one may obtain an accurate approximation of its dynamics by modelling the dynamics of the first few moments. Wirtz and Eckhardt (1996) proposed the Effective Variable (EV) approach, which assumes the trait distribution can be approximated by a normal distribution; they subsequently take its variance constant and evolve the mean. Similarly, Norberg et al. (2001) evolve the mean and variance of an arbitrary univariate trait distribution using simulation-based parameterizations of its skewness and kurtosis. For the present phytoplankton SID, we have obtained good results by assuming a (bivariate) lognormal trait distribution and evolving its mean and covariances: depth- and time-averaged deviations from the present results equalled 1.2% for structural biomass, 6.6% for the mean, and 10.3% for the covariances, measured relative to the respective maximum ranges (in preparation). Although reduction of the trait distribution to the first few moments can in theory eliminate interesting dynamics (in particular multimodality), we deem it a promising direction for further expansion of the SID concept. Given that the number of state variables necessary for discretized trait distributions increases exponentially with the number of traits, it will certainly prove indispensable for modelling systems with more than two traits.

The phytoplankton SID integrates separate theories dealing with species diversity and succession: It demonstrates changes in species composition with depth as proposed by the concept of a shade flora, as well as seasonal succession in time in line with Margalef (1978). It does so with a minimum of parameters (4), and as such might be said to successfully illustrate the potential of biodiversity-based approaches to aquatic ecosystem modelling. Obviously, the present model lacks a wealth of physiological detail (Flynn 2001; Geider et al. 1998; Pahlow 2005), and will not reproduce some features that emerge from detailed laboratory studies (e.g., photoinhibition, nutrient buffering). However, for understanding of aquatic ecosystems as a whole, we believe models will benefit more from improved representations of biodiversity and succession than from more accurate representations of (partially species-specific) physiological processes. The SID approach could be a starting point for a next generation of ecosystem models.
2. A biodiversity-inspired approach to aquatic ecosystem modeling

2.5 Appendix: water column model

The phytoplankton SID is hosted within a vertically structured model for the ocean water column (Burchard et al. 2006; Burchard et al. 1999). Biota experience variation in time and depth through two variables: Light intensity and (turbulent) diffusivity. Details of the physical model are described in (Burchard et al. 1999), whereas a good overview of the generic model and our particular configuration can be found in (Allen et al. 2004); therefore, we will limit the discussion of the physical model here to a qualitative description.

Light intensity (in W m\(^{-2}\)) is calculated according to astronomical formulae (Allen et al. 2004) using the geographical location and the local date and time; both diurnal and seasonal variation are accounted for. Solar radiation is attenuated by clouds before reaching the surface, which is quantified through an imposed time-varying cloud cover; thus we take unpredictable high-frequency variation in weather conditions into account. Of all short-wave solar radiation reaching the surface, a fixed fraction (38\%) is assumed to be photosynthetically active radiation (PAR). This fraction is attenuated as it penetrates the water column, using an extinction length of 20 m; this gives rise to the vertical gradient in PAR.

Turbulence is produced in unstable density gradients (buoyancy production) and flow velocity gradients (shear production), and decays in stable density gradients. It is by nature unstable: Viscous friction causes continuous dissipation of turbulent eddies into heat. To describe turbulence in the water column we apply the well-known \( k-\epsilon \) model, which quantifies turbulence by its total kinetic energy \( k \) and dissipation rate \( \epsilon \), and describes the dynamics of these quantities with parameterizations of the effects of buoyancy and shear. Ultimately turbulent quantities are used to derive an effective, turbulent diffusivity \( D \), which exclusively controls transport of physical quantities (temperature, salinity) as well as nutrient and biota.

We explicitly describe the vertical structure of the water column, implicitly assuming all physical variables are horizontally homogeneous. Thus turbulence is exclusively controlled by vertical gradients in density and flow velocity, which in turn are affected by surface- and bottom boundary conditions and turbulent mixing. Density gradients combine the contributions of temperature and salinity, and as such are mediated by surface heat exchange, evaporation, precipitation, and absorption of light by water (the latter across the entire column). Flow velocity gradients are mediated by surface wind stress and bottom friction. In our setup, effective surface boundary conditions directly follow from weather conditions: Transport of heat and momentum across the surface is calculated according to Kondo (1975) from time-varying meteorological variables air temperature, air humidity, air pressure, wind speed, wind direction, and net precipitation. Through this link, the amount of turbulence will come to reflect seasonal and non-seasonal variation in weather conditions; this allows the model to reproduce biologically relevant effects such as summer stratification and formation of a well-mixed layer extending beyond the euphotic zone in autumn/winter.
The dynamic behaviour of the structural biomass concentration of phytoplankton population \( i \) at some depth \( z \) is now given by

\[
\frac{\partial V_i}{\partial t} = \frac{1}{1 + m_{L,i} + m_{N,i}} \left( \frac{1}{1 + \left( \frac{m_{L,i} X_L}{K_L} \right)^{-1}} + \frac{1}{\left( \frac{m_{N,i} X_N}{K_N} \right)^{-1}} - \left( \frac{m_{L,i} X_L}{K_L} + m_{N,i} X_N \right)^{-1} \right) 
- \left( 1 + m_{L,i} + m_{N,i} \right) V_i k 
+ \kappa D \left( V_{i,ref} - V_i \right) 
+ \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} V_i \right),
\]

in which \( D \) denotes the (turbulent) diffusivity calculated by the physical model, \( k \) denotes the immigration rate relative to the diffusivity, and \( V_{i,ref} \) the reference structural biomass concentration of species \( i \) (equal to its initial concentration). The first line denotes biomass production (\( J_{V,i} \), cf. Eqs. 1 and 2), the second line biomass turnover due to maintenance (\( J_{VM,i} \), cf. Eq. 3), the third line immigration, and the fourth line vertical diffusion. Note that depth- and time-dependencies of \( V, X_L, X_N \) and \( D \) are suppressed. Nutrient dynamics mirror the dynamics of the total phytoplankton biomass (structural- as well as harvesting biomass) summed over all species, and also incorporate contributions from immigration and diffusion; the dynamics of the nutrient concentration at depth \( z \) thus equal

\[
\frac{\partial X_N}{\partial t} = - \sum_i V_i \frac{\partial}{\partial t} \frac{1}{1 + \left( \frac{m_{L,i} X_L}{K_L} \right)^{-1}} + \frac{1}{\left( \frac{m_{N,i} X_N}{K_N} \right)^{-1}} - \left( \frac{m_{L,i} X_L}{K_L} + m_{N,i} X_N \right)^{-1} 
+ \sum_i V_i \left( 1 + m_{L,i} + m_{N,i} \right) k 
+ \kappa D \left( X_{N,ref} - X_N \right) 
+ \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} X_N \right),
\]

in which \( X_{N,ref} \) denotes the reference nutrient concentration (equal to the initial concentration). The first line denotes the change due to biological activity, the second line immigration, and the third line vertical diffusion. Both the surface and bottom of the water column are closed for mass, which translates into the following boundary conditions

\[
D \frac{\partial}{\partial z} V_i \bigg|_{z=0} = 0 \quad D \frac{\partial}{\partial z} V_i \bigg|_{z=x_{max}} = 0 \\
D \frac{\partial}{\partial z} X_N \bigg|_{z=0} = 0 \quad D \frac{\partial}{\partial z} X_N \bigg|_{z=x_{max}} = 0,
\]
with $z_{\text{max}}$ denoting the depth of the column. These conditions specify that the fluxes of structural mass and nutrient across the surface ($z = 0$) and the bottom ($z = z_{\text{max}}$) equal zero; note that this implies that fluxes of harvesting biomasses across the interfaces also equal zero.

We configure the physical model to describe the site of the Bermuda Atlantic Time-series Study (BATS), at 31.7° north, 64.2° west. This location has been subject to intensive study in past and present (Steinberg et al. 2001), which has produced detailed knowledge of the dynamics of many physical and several biological variables in time and depth. Particularly valuable to us are the monthly depth profiles of temperature and salinity from 1988 onwards; these serve to initialize the column as well as allow us to judge the accuracy of the results of physical model. All necessary weather conditions are taken from the 6-hourly ERA-40 re-analysis dataset (Uppala et al. 2005), obtained from the ECMWF Data Server (http://www.ecmwf.int). The column model is restricted to the top 400 m of the BATS site, using a vertical grid of 100 layers and increasing resolution near the surface (the layer thickness decreases from 8.3 m to 0.6 m). The depth of 400 m was chosen for accurate resolution of the mixed layer (which never reaches beyond depths of 250 m) without interference of the bottom boundary conditions; the depth is more than sufficient for resolution of the primary producers, which are not found below the 200 m level (Steinberg et al. 2001).

2.6 References


2. A biodiversity-inspired approach to aquatic ecosystem modeling


3 An approximation for succession-based dynamics of trait distributions

Unpublished manuscript

Abstract
We consider the behaviour of a community of species, modelled as a probability distribution of one or more continuous traits. This community is embedded in a spatial context with advection and diffusion, exposed to temporally variable environmental conditions. The trait distribution is characterized by a few key variables – the distributional moments – which then are evolved in time and space. While different types of moments could be used to characterize a distribution, it is shown that only the raw moments of the biomass distribution can be used directly in an advection-diffusion context. The system is therefore completely expressed in terms of this type of moments. Subsequently, contributions of immigration and population growth to the moment dynamics are considered. Because the effect of population growth cannot be described exactly without complete knowledge on the shape of the trait distribution, a moment closure technique is used to derive an efficient approximation based on lower moments only.
3. An approximation for succession-based dynamics of trait distributions

3.1 Introduction

We consider a community of species modelled as a probability distribution of multiple traits, in a spatial context with advection and diffusion, exposed to temporally variable environmental conditions. For the sake of computational efficiency, the trait distribution is characterized by a few key variables – the distributional moments – which can then be evolved in time and space. By considering spatial variability and multiple correlated traits, this study expands on earlier studies that considered a single trait (Norberg et al. 2001), multiple uncorrelated traits (Wirtz and Eckhardt 1996), and multiple correlated traits (Savage et al. 2007) in non-spatial setting.

Different types of distributional moments can be used to characterize a distribution. A common choice is the combination of the total biomass, mean and covariances of the distribution. However, it is shown that an advection-diffusion context poses specific requirements on the behaviour of the state variables of the system, and that only one category of distributional moments (raw moments of the biomass distribution) meets these requirements. The system is therefore expressed completely in terms of this type of moments.

Subsequently the contributions of immigration (cf. Norberg et al. 2001; Savage et al. 2007) and population growth to the dynamics of distributional moments are discussed. The change in moments induced by population growth is first expressed in terms of the complete set of multivariate moments (Savage et al. 2007). Subsequently efficient approximations is introduced based on normal- and log-normal moment closures.

3.2 Notation

Wherever possible, we will follow the derivation and notation of Norberg et al. (2001). One notable exception is the use of a Taylor series expansion of the population growth rate: whereas Norberg et al. use the full expansion throughout the derivation, and finally approximate by neglecting higher order terms, we apply this approximation immediately. This was done solely to improve readability; anyone with considerable amounts of paper at his disposal and a persistent disposition would be able to follow our derivation with higher order terms included. Higher-order formulations in compact, non-conventional notation may also be found in Savage et al. (2007).

When integrating over an $n$-dimensional distribution $f(x)$ with variates combined in vector $x \in \mathbb{R}^n$, we will use $\int_a^b f(x)dx$, $a, b \in \mathbb{R}^n$ to denote $\int_{a_1}^{b_1} \int_{a_2}^{b_2} \ldots \int_{a_n}^{b_n} f(x_1, x_2, \ldots, x_n)dx_1 dx_2 \ldots dx_n$.

Like Norberg et al. and Savage et al., we use $M$ to denote moments about the mean. However, we define the meaning of subscripts of the moment symbol differently, to simplify notation when the typical number of variates is large and the order of moments is low. This allows us to use conventional notation throughout the study (cf. Savage et al.). First, we define a $j^{th}$ order raw moment (i.e., moment about zero) of an $n$-variate probability distribution $f(x)$ as
3.3 The problem

Let us consider a community of species, each species quantified by a population density or concentration. Species can differ in quantifiable characteristics, which we combine in trait vector \( \mathbf{s} \in \mathbb{R}^S \). By definition, any unique trait vector \( \mathbf{s} \) defines a species. All species are placed in a one-dimensional spatial setting, e.g., a water column; \( z \) will be used to denote the spatial coordinate. The concentration of species is governed by local biological processes (e.g., population growth) and immigration of new individuals, as well as “advection” (transport of the medium as well as sinking and floating) and diffusion.

The dynamic behaviour of any single population with trait value \( s \) is described by

\[
\frac{\partial}{\partial t} C(s) = F(s) + I(s) - \frac{\partial}{\partial z} \left( wC(s) \right) + \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} C(s) \right),
\]

with the first term on the right-hand side describing local biological processes, the second describing immigration, the third advection, and the fourth diffusion. \( C, F, I, w \) and \( D \) may all depend on time and depth; these dependencies are suppressed for the sake of readability. Note that we thus explicitly allow for the advection velocity (or sinking/floating rate) and (turbulent) diffusion coefficient to be depth-dependent.

From this point on, we will consider traits to be continuous variables. Rather than considering distinct species with unique \( \mathbf{s} \in \mathbb{R}^S \), we will consider the \( S \)-dimensional trait value distribution, a function of \( \mathbf{s} \). Let the concentration of biomass in all species with a trait vector \( \mathbf{s} \in [a, b] \) equal

\[
\int_a^b c(s) \, ds.
\]
We will assume that this integral exists, and is positive, for \( a_i \to -\infty, b_i \to \infty, \forall i \); in other words, we assume the distribution of biomass as a function of trait values can be described by a valid probability distribution. Then the total biomass is given by

\[
C_T = \int c(s) ds, \tag{3.2}
\]

and the probability distribution (its integral over the whole trait value domain equal to 1) for the trait value is given by \( c(s)/C_T \). The dynamics of any point in the trait distribution (dimension: biomass per trait per time) are given by (3.1), with \( C(s) \) replaced by \( c(s) \) and \( f(s) \) replaced by \( l(s) \):

\[
\frac{\partial}{\partial t} c(s) = f(s) + \frac{\partial}{\partial s} \left( wc(s) \right) + \frac{\partial}{\partial s} \left( D \frac{\partial}{\partial s} c(s) \right). \tag{3.3}
\]

### 3.4 Distributional moments

Rather than evolving the biomass distribution \( c(s) \) through discretization of trait space \( s \), as in chapter 2, we now develop the dynamics of a select set of statistics of the distribution in order to capture the maximum of dynamics of the distribution combined with a minimum of computational effort. An intuitive choice of distribution characteristics are the distributional moments, e.g., the mean and covariances. We will first define several different types of moments, which are interchangeable in characterizing the distribution. Subsequently we will study the behaviour of the different types of moments in a context with advection and diffusion, and conclude that only one type of moment is suited to be embedded in advection-diffusion modelling frameworks.

The probability distribution of traits equals \( c(s)/C_T \), which implies that its \( j \)th order raw moment (e.g., the mean if \( f = 1 \)) and its \( j \)th order central moment (e.g., the covariance if \( f = 2 \)) are respectively given by

\[
M'_{c_1,...,c_j} = \frac{1}{C_T} \int \left( \prod_{i=1}^j s_{c_i} \right) c(s) ds
\]

\[
M_{c_1,...,c_j} = \frac{1}{C_T} \int \left( \prod_{i=1}^j s_{c_i} - \bar{s}_{c_i} \right) c(s) ds, \text{ with } c_i \in \{1, \ldots, S\} \tag{3.4}
\]

It will also prove useful to consider the raw moments of the biomass distribution \( c(s) \). These directly relate to the raw moments of the probability distribution as

\[
\int \left( \prod_{i=1}^j s_{c_i} \right) c(s) ds = C_T M'_{c_1,\ldots,c_j}, \text{ with } c_i \in \{1, \ldots, S\}. \tag{3.5}
\]

For \( j = 0 \) the product term is defined to equal 1, thus yielding the total biomass \( C_T \).

Conversions between different types of moments are well-defined. If the total biomass \( C_T \) is known, it is trivial to calculate the moments of the biomass distribution \( c(s) \) from the moments of the trait probability distribution \( c(s)/C_T \) and vice versa. Similarly, if the distributional mean is known, the complete set of raw moments can be
calculated from the complete set of central moments and vice versa (Johnson and Kotz 1972). Thus to characterize the (evolution of) the trait distribution, we have some freedom to choose moments (raw or central, of the probability distribution or of the biomass distribution) that behave most conveniently for our purposes.

The combination of the mean and covariances (and higher order central moments) arguably provides a most intuitive characterization of the trait distribution. Also, these moments appear naturally in expressions for the effect of population growth on moment dynamics (Norberg et al. 2001). Given (3.4), the mean and covariances of the trait distribution equal

\[
\bar{s}_i = M_i' = \frac{1}{c_T} \int s_i c(s) ds
\]

\[
M_{ij} = \frac{1}{c_T} \int (s_i - \bar{s}_i)(s_j - \bar{s}_j) c(s) ds'
\] with \(i,j \in \{1, \ldots, S\}\)

(3.6)

Covariances may be rewritten in terms of raw moments:

\[
M_{ij} = \frac{1}{c_T} \int s_is_j c(s) ds - \bar{s}_i \bar{s}_j = M_{ij}' - \bar{s}_i \bar{s}_j.
\] (3.7)

Analogous expressions for higher central moments, e.g. skewness and kurtosis, can also be constructed (Johnson and Kotz 1972).

### 3.5 Generic time derivatives

Given the biomass distribution \(c(s)\) and its time derivative (3.3), we can now formulate the time derivatives of the distributional moments. Starting with the generic raw moments (3.5) of the biomass distribution

\[
\frac{\partial}{\partial t} (C_T M_{c_1c_2\ldots c_J}) = \frac{\partial}{\partial t} \int (\Pi_{i=1}^J s_{c_i}) c(s) ds = \int (\Pi_{i=1}^J s_{c_i}) \frac{\partial}{\partial t} c(s) ds
\] (3.8)

Through the quotient rule, this renders for the raw moments of the trait probability distribution

\[
\frac{\partial}{\partial t} M_{c_1c_2\ldots c_j} = \frac{1}{c_T} \left( \frac{\partial}{\partial t} \left( C_T M'_{c_1c_2\ldots c_j} \right) - M'_{c_1c_2\ldots c_j} \frac{\partial}{\partial t} C_T \right)
\]

\[
= \frac{1}{c_T} \left( \int (\Pi_{i=1}^J s_{c_i}) \frac{\partial}{\partial t} c(s) ds - M'_{c_1c_2\ldots c_j} \frac{\partial}{\partial t} C_T \right)
\] (3.9)

A generic expression for the time derivative of central moments exists but is more complex; for our purposes the time derivative of the covariance suffices, which we derive separately below.
3. An approximation for succession-based dynamics of trait distributions

The dynamics of the total biomass (3.2), i.e., the 0th order moment of the biomass distribution, equal

$$\frac{\partial}{\partial t} C_T = \frac{\partial}{\partial t} \int c(s) ds = \int \frac{\partial}{\partial t} c(s) ds$$  \hspace{1cm} (3.10)

The dynamics of the mean (3.6) are given by (3.9) if $\frac{\partial}{\partial t} \bar{s}_i = 1$:

$$\frac{\partial}{\partial t} \bar{s}_i = \frac{1}{C_T} \left( \frac{\partial}{\partial t} (C_T \bar{s}_i) - \bar{s}_i \frac{\partial}{\partial t} C_T \right),$$  \hspace{1cm} (3.11)

in which (3.8) and (3.10) might be substituted to express the dynamics of the mean in terms of the trait distribution and its derivatives alone. Working from (3.7), the dynamics of the covariance equal

$$\frac{\partial}{\partial t} M_{ij} = \frac{\partial}{\partial t} M'_{ij} - \bar{s}_i \frac{\partial}{\partial t} \bar{s}_j - \bar{s}_j \frac{\partial}{\partial t} \bar{s}_i,$$  \hspace{1cm} (3.12)

in which (3.9) and (3.11) might be substituted to express the covariance dynamics in terms of the trait distribution and its derivatives alone.

It is fairly easy to check that all moment derivatives (3.8)-(3.12) are linear maps of the time derivative of $C_T$, which implies they satisfy the additivity condition:

$$\frac{\partial}{\partial t} m \bigg|_{c(s)=a(s)+b(s)} = \frac{\partial}{\partial t} m \bigg|_{c(s)=a(s)} + \frac{\partial}{\partial t} m \bigg|_{c(s)=b(s)},$$

for $m = C_T M c_{ij} \bar{s}_i C_T \bar{s}_j$. This is a useful property, as it means that the effects of the different components of (3.3) (population dynamics, immigration, advection, diffusion) on the dynamics of the total biomass, mean and covariances can be determined individually, and summed to produce complete moment derivatives as a last step.

### 3.6 Advection and diffusion

The combination of the mean and central moments (e.g., covariances) provides an intuitive and attractive characterization of the trait distribution. However, in a context that includes advection and diffusion, the mean and central moments are not necessarily the most convenient choice of state variables. In selecting the moments $m$ to evolve (raw or central moments, of the biomass distribution or the trait probability distribution) we take interest in the following properties:

$$\frac{\partial}{\partial t} m \bigg|_{c(s)=a(s)} = \frac{\partial}{\partial x} (wm),$$

$$\frac{\partial}{\partial t} m \bigg|_{c(s)=a(s)} = \frac{\partial}{\partial x} \left( D \frac{\partial}{\partial x} m \right),$$  \hspace{1cm} (3.13)
which simply state that the distribution statistic \( m \) must behave as a standard tracer if distribution dynamics are governed by advection and diffusion, respectively. This is a requirement if the model is to directly embedded in an advection-diffusion framework that numerically solves advection and diffusion of variables separately and independently (e.g. Burchard et al. 1999). This possibility for direct embedding is important, as it allows the advection-diffusion components within the model to be solved with existing numerical schemes. If the model included state variables that do not behave as a standard tracers, it would be necessary to develop custom numerical schemes for advection and diffusion – a monumental task indeed.

It may be noted that the first condition in (3.13) could be relaxed to

\[
\frac{\partial}{\partial t} m \bigg|_{\frac{\partial c(s)}{\partial t} = w \frac{\partial c(s)}{\partial z}} = w \frac{\partial}{\partial z} m,
\]

if the advection rate \( w \) were independent of depth. In three spatial dimensions, the same applies if the advection-governed transport is divergence-free. This “divergence-free” condition is usually met by transport of passive tracers in hydrodynamic models, in which case the advection equation describes the effect of flow of the (incompressible) medium only. However, it is not necessarily met if factors other than the flow contribute to the “advection” rate \( w \), as these contributions may vary in space. This occurs for instance if the transported quantities sink with a rate that is depth-dependent, which is not unusual in the biogeochemical models that are in use at present. Therefore, we will not require the advection process to be divergence-free.

### 3.6.1 Raw moments of the biomass distribution

For the isolated advection component of (3.3), the dynamics of the raw moments as given by (3.8) equal

\[
\frac{\partial}{\partial t} C_T M'_c = - \int \left( \prod_{i=1}^{j} s_{c_i} \right) \frac{\partial}{\partial z} (w c(s)) ds.
\]

Expanding according to the product rule yields

\[
\frac{\partial}{\partial t} C_T M'_{c_1,...,c_j} = -w \int \left( \prod_{i=1}^{l} s_{c_i} \right) \frac{\partial}{\partial z} c(s) ds - \int \left( \prod_{i=1}^{j} s_{c_i} \right) c(s) ds \frac{\partial}{\partial z} w,
\]

as \( w \) and \( \partial w / \partial z \) do not depend on \( s \). Substituting the raw moment (3.5) and its vertical gradient

\[
\frac{\partial}{\partial t} C_T M'_{c_1,...,c_j} = -w \frac{\partial}{\partial z} \left( C_T M'_{c_1,...,c_j} \right) - C_T M'_{c_1,...,c_j} \frac{\partial}{\partial z} w = -\frac{\partial}{\partial z} \left( w C_T M'_{c_1,...,c_j} \right) \tag{3.14}
\]
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This succinctly demonstrates that raw moments of the biomass distribution behave as standard tracers with respect to advection.

For the isolated diffusion component of (3.3), the dynamics of the raw moments as given by (3.8) equal

\[
\frac{\partial}{\partial t} C_{T_1 \cdots T_j} = \int \left( \prod_{i=1}^{j} s_{c_{i}} \right) \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} c(s) \right) ds.
\]

Expanding according to the product rule yields

\[
\frac{\partial}{\partial t} C_{T_1 \cdots T_j} = D \int \left( \prod_{i=1}^{j} s_{c_{i}} \right) \frac{\partial^2}{\partial z^2} c(s) ds - \int \left( \prod_{i=1}^{j} s_{c_{i}} \right) \frac{\partial}{\partial z} c(s) ds \frac{\partial D}{\partial z},
\]

as \( D \) and \( \partial D/\partial z \) do not depend on \( s \). Substituting gradients of the raw moment (3.5)

\[
\frac{\partial}{\partial t} C_{T_{i_1} \cdots T_{i_j}} = D \frac{\partial^2}{\partial z^2} \left( C_{T_{i_1} \cdots T_{i_j}} \right) + \frac{\partial}{\partial z} D \frac{\partial}{\partial z} \left( C_{T_{i_1} \cdots T_{i_j}} \right) = \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} C_{T_{i_1} \cdots T_{i_j}} \right), \tag{3.15}
\]

demonstrating that raw moments of the biomass distribution behave as standard tracers with respect to diffusion as well.

### 3.6.2 Total biomass

The total biomass equals the 0th order raw moment of the biomass distribution. For the isolated advection component of (3.3), the dynamics of the total biomass are therefore given by (3.14) if \( j = 0 \):

\[
\frac{\partial}{\partial t} C_T = - \frac{\partial}{\partial z} (wc_T). \tag{3.16}
\]

Similarly, for the isolated diffusion component of (3.3), the dynamics of the total biomass are given by (3.15) if \( j = 0 \):

\[
\frac{\partial}{\partial t} C_T = \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} C_T \right). \tag{3.17}
\]

As all raw moments of the biomass distribution, the total biomass therefore behaves like a standard tracer with respect to advection and diffusion.
3.6.3 Raw moments of the trait probability distribution

For the isolated diffusion component of (3.3), we can substitute time derivatives of
the raw moment (3.14) and the total biomass (3.16) in (3.9), to obtain

\[ \frac{\partial}{\partial t} M'_{c_{1-c_j}} = - \frac{1}{C_T} \left( \frac{\partial}{\partial z} \left( wC_T M'_{c_{1-c_j}} \right) - M'_{c_{1-c_j}} \frac{\partial}{\partial z} \left( wC_T \right) \right) \]

Applying the product rule renders

\[ \frac{\partial}{\partial t} M'_{c_{1-c_j}} = - \frac{1}{C_T} \left( M'_{c_{1-c_j}} \frac{\partial}{\partial z} \left( wC_T \right) + wC_T \frac{\partial}{\partial z} M'_{c_{1-c_j}} - M'_{c_{1-c_j}} \frac{\partial}{\partial z} \left( wC_T \right) \right) = -w \frac{\partial}{\partial z} M'_{c_{1-c_j}} \tag{3.18} \]

This is similar but not identical to the \(- \frac{\partial}{\partial z} \left( w M'_{c_{1-c_j}} \right) / \partial z\) that would be expected for
standard tracers. Specifically, raw moments of the trait probability distribution are
not sensitive to spatial variation of \(w\), i.e., to the divergence of the flow field. In
practice, that means that raw moments of the trait probability distribution (e.g., the
mean trait value) would not be affected by an increasing or decreasing sinking rate,
whereas normal tracers such as biomass would be. It also implies that these raw
moments cannot be incorporated directly in most hydrodynamics models, unless
numerical advection schemes are adapted to ensure that these moments are not
affected by the divergence of the advection process.

For the isolated diffusion component of (3.3), we can substitute time derivatives of
the raw moment (3.15) and the total biomass (3.17) in (3.11), to obtain

\[ \frac{\partial}{\partial t} M'_{c_{1-c_j}} = \frac{1}{C_T} \left( \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} \left( C_T M'_{c_{1-c_j}} \right) \right) - M'_{c_{1-c_j}} \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} C_T \right) \right) \]

Applying the product rule repeatedly and collecting terms containing \(D\) and \(\partial D / \partial z\)

\[ \frac{\partial}{\partial t} M'_{c_{1-c_j}} = \frac{1}{C_T} \left( C_T \frac{\partial}{\partial z} D \frac{\partial}{\partial z} M'_{c_{1-c_j}} + D \left( C_T \frac{\partial^2}{\partial z^2} M'_{c_{1-c_j}} + 2 \frac{\partial}{\partial z} C_T \frac{\partial}{\partial z} M'_{c_{1-c_j}} \right) \right) \]

Expanding yields

\[ \frac{\partial}{\partial t} M'_{c_{1-c_j}} = \frac{\partial}{\partial z} D \frac{\partial}{\partial z} M'_{c_{1-c_j}} + D \frac{\partial^2}{\partial z^2} M'_{c_{1-c_j}} + 2 \frac{\partial}{\partial z} C_T \frac{\partial}{\partial z} M'_{c_{1-c_j}} \frac{\partial}{\partial z} C_T \]

\[ = \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} M'_{c_{1-c_j}} \right) + 2 \frac{\partial}{\partial z} C_T \frac{\partial}{\partial z} M'_{c_{1-c_j}} \]

\[ \tag{3.19} \]

This equals \(\partial (D \frac{\partial M'_{c_{1-c_j}}}{\partial z}) / \partial z\) only if \(\frac{\partial M'_{c_{1-c_j}}}{\partial z} / \partial z = 0\) or \(\frac{\partial C_T}{\partial z} = 0\), i.e., if the
value of \(M'_{c_{1-c_j}}\) and/or \(C_T\) is homogeneous across the column. In non-trivial scenarios
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this will not be the case. Thus, raw moments of the trait probability distribution do not behave as a standard tracer in a context with diffusion.

3.6.4 Mean

The mean equals the 1st order raw moment of the trait probability distribution. For the isolated advection component of (3.3), the dynamics of the total biomass are therefore given by (3.18) if \( j = 1 \): 

\[
\frac{\partial}{\partial t} \bar{s}_i = -w \frac{\partial}{\partial z} \bar{s}_i \tag{3.20}
\]

Similarly, for the isolated diffusion component of (3.3), the dynamics of the total biomass are therefore given by (3.19) if \( j = 1 \): 

\[
\frac{\partial}{\partial t} \bar{s}_i = \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} \bar{s}_i \right) + 2 \frac{\partial}{\partial z} \left( \frac{\partial}{\partial z} C_T \bar{s}_i \right) \tag{3.21}
\]

As all raw moments of the trait probability distribution, the mean therefore does not behave as a standard tracer in a context with advection and diffusion.

3.6.5 Covariances

For the isolated advection component of (3.3), we can substitute time derivatives of the 2nd order raw moment of the trait probability distribution, (3.18), and the mean (3.20) in (3.12), to obtain

\[
\frac{\partial}{\partial t} M_{ij} = -w \left( \frac{\partial}{\partial z} M_{ij}' - \bar{s}_i \frac{\partial}{\partial z} \bar{s}_j - \bar{s}_j \frac{\partial}{\partial z} \bar{s}_i \right)
\]

Substituting \( M_{ij}' \) by \( M_{ij} + \bar{s}_i \bar{s}_j \) renders

\[
\frac{\partial}{\partial t} M_{ij} = -w \left( \frac{\partial}{\partial z} \left( M_{ij} + \bar{s}_i \bar{s}_j \right) - \bar{s}_i \frac{\partial}{\partial z} \bar{s}_j - \bar{s}_j \frac{\partial}{\partial z} \bar{s}_i \right) = -w \frac{\partial}{\partial z} M_{ij}
\]

Thus, as for the raw moments of the trait probability distribution, covariances behave as standard tracers with respect to advection only if the transport is divergence-free, i.e., \( \partial w / \partial z = 0 \).

For the isolated diffusion component of (3.3), we can substitute time derivatives of the 2nd order raw moment of the trait probability distribution, (3.19), and the mean (3.21) in (3.12), to obtain

\[
\frac{\partial}{\partial t} M_{ij} = \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} M_{ij}' \right) - \bar{s}_i \frac{\partial}{\partial z} \bar{s}_j \left( D \frac{\partial}{\partial z} \bar{s}_j \right) - \bar{s}_j \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} \bar{s}_i \right) + 2 \frac{\partial}{\partial z} \left( \frac{\partial}{\partial z} C_T \bar{s}_i \right) \bar{s}_j \frac{\partial}{\partial z} \bar{s}_i \frac{\partial}{\partial z} C_T
\]
Substituting $M'_{ij}$ by $M_{ij} + \tilde{s}_i\tilde{s}_j$ and applying the product rule renders

$$\frac{\partial}{\partial t} M_{ij} = \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} M_{ij} \right) + \frac{\partial}{\partial z} \left( D\tilde{s}_i \frac{\partial}{\partial z} \tilde{s}_j \right) + \frac{\partial}{\partial z} \left( D\tilde{s}_j \frac{\partial}{\partial z} \tilde{s}_i \right) - \tilde{s}_i \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} \tilde{s}_j \right) - \tilde{s}_j \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} \tilde{s}_i \right) + 2 \frac{D}{C_T} \frac{\partial}{\partial z} \left( M_{ij} \right) \frac{\partial}{\partial z} C_T.$$

Applying the product rule to the second and third term yields

$$\frac{\partial}{\partial t} M_{ij} = \frac{\partial}{\partial z} \left( D \frac{\partial}{\partial z} M_{ij} \right) + 2D \left( \frac{\partial}{\partial z} \tilde{s}_i \frac{\partial}{\partial z} \tilde{s}_j + \frac{1}{C_T} \frac{\partial}{\partial z} C_T \frac{\partial}{\partial z} M_{ij} \right).$$

The first term in this summation is a normal diffusion expression. Due to the presence of the second term, however, covariances do not behave as standard tracers with respect to diffusion.

### 3.6.6 Choosing the type of moments to evolve

The mean and covariances of the trait distribution are intuitive properties to focus on. However, the above derivations demonstrate that only raw moments of the biomass distribution meet condition (3.13), i.e., they behave as standard tracers with respect to advection and diffusion. These moments can thus be embedded directly in frameworks that numerically solve advection-diffusion equations of tracers. Therefore, it is often most straightforward to evolve raw moments of the biomass distribution, and transform these to the mean and central higher order moments of the trait distribution only where needed. This approach is followed in the present study; the system is completely expressed in terms of raw moments of the biomass distribution. From these moments the actual mean and covariances are calculated when needed, e.g., for calculating the effect of population growth on distribution statistics (see below) and for presentation of easily interpretable output statistics.

### 3.7 Immigration

For the isolated immigration component of (3.3), the dynamics of the raw moments (3.8) of the biomass distribution equal

$$\frac{\partial}{\partial t} C_T M'_{c_1-c_j} = \int \left( \prod_{i=1}^{j} \delta_{c_i} \right) i(s) ds.$$

Similar to Norberg et al. (2001), we now introduce the moments of the distribution of immigration species

$$C_T^{(i)} M'_{c_1-c_j} = \int \left( \prod_{i=1}^{j} \delta_{c_i} \right) i(s) ds,$$
which have the dimension of the corresponding raw moment $C_T M'_{c_{i+1}, c_{j}}$ per time. If immigration is described as the product of an external trait distribution $e(s)$ and a trait-independent immigration rate $i(s) = d e(s)$, we obtain

$$\frac{d}{dt} C_T M'_{c_{i+1}, c_{j}} = C_T M^{(i)}_{c_{i+1}, c_{j}} = d \int \left( \prod_{l=1}^{l-1} s_{c_l} \right) e(s) ds = d C_T^{(e)} M^{(e)}_{c_{i+1}, c_{j}}$$

(3.22)

with $C_T^{(e)}$ denoting the total biomass of the immigrating community, and $M^{(e)}_{c_{i+1}, c_{j}}$ denoting the raw moment of the associated trait probability distribution. Thus raw moments of the biomass distribution behave normal with respect to immigration: if species from some external distribution $e(s)$ immigrate with rate $i(s)$, the local raw moments of the biomass distribution increase with $d$ times the corresponding moment of $e(s)$ as well.

From (3.11), (3.12) and (3.22) one could might also derive the change in the mean and covariances as a result of immigration (Norberg et al. 2001; Savage et al. 2007); however, as we express the complete system in terms of moments of the biomass distribution this is not needed for the present study.

### 3.8 Population growth

Let us assume that the population dynamics component of (3.3) is proportional to biomass, i.e.,

$$f(s) = r(s) c(s)$$

(3.23)

This would be the case for many models of population growth, in which the growth rate is proportional to population size. It may be noted that this can includes emigration, in the common scenario where a fraction of the resident population emigrates per unit time. In isolation, the population dynamics component of the dynamics of the trait distribution then equals

$$\frac{d}{dt} c(s) = r(s) c(s),$$

(3.24)

noting that both $c$ and $r$ may depend on time and depth.

#### 3.8.1 Total biomass

For population growth equation (3.24), the dynamics of the total biomass as given by (3.10) are given by

$$\frac{d}{dt} C_T = \int r(s) c(s) ds.$$  

(3.25)
To solve the integral of population growth, we first approximate the specific growth rate \( r(\mathbf{s}) \) by a Taylor series about the average trait value \( \bar{\mathbf{s}} = (\bar{s}_i, \ldots, \bar{s}_S)' \), rendering

\[
r(\mathbf{s}) = \sum_{i=0}^{\infty} \frac{1}{i!} (\mathbf{s} - \bar{\mathbf{s}}) \cdot \frac{d^i}{d\mathbf{s}^i} r(\mathbf{s})\big|_{\mathbf{s} = \bar{\mathbf{s}}},
\]

(3.26)

Here, it is worth noting that \( (\mathbf{s} - \bar{\mathbf{s}}) \cdot \frac{d}{d\mathbf{s}} = \sum_{i=1}^{S} (s_i - \bar{s}_i) \frac{\partial}{\partial s_i} \).

We can use (3.26) to approximate the population growth term in (3.25):

\[
\frac{\partial}{\partial t} C_T = \int c(\mathbf{s}) \sum_{i=0}^{\infty} \frac{1}{i!} \left[ (\mathbf{s} - \bar{\mathbf{s}}) \cdot \frac{d}{d\mathbf{s}} \right] r(\mathbf{s})\bigg|_{\mathbf{s} = \bar{\mathbf{s}}} \right) d\mathbf{s}
\]

Evaluated up to the second order term:

\[
\frac{\partial}{\partial t} C_T \approx \int c(\mathbf{s}) \left( \left. \frac{r(\mathbf{s})}{(\mathbf{s} - \bar{\mathbf{s}})^T} \cdot \frac{d}{d\mathbf{s}} r(\mathbf{s}) \right|_{\mathbf{s} = \bar{\mathbf{s}}} + \frac{1}{2} (\mathbf{s} - \bar{\mathbf{s}})^T H(\mathbf{s}) \right|_{\mathbf{s} = \bar{\mathbf{s}}} (\mathbf{s} - \bar{\mathbf{s}}) \right) d\mathbf{s}
\]

(3.27)

With \( H(\mathbf{s})\big|_{\mathbf{s} = \bar{\mathbf{s}}} \) denoting the Hessian matrix with elements \( H_{ij}(\mathbf{s}) = \left. \frac{\partial^2}{\partial s_i \partial s_j} r(\mathbf{s}) \right|_{\mathbf{s} = \bar{\mathbf{s}}} \), evaluated in the mean trait value \( \bar{\mathbf{s}} \), and \( (\mathbf{s} - \bar{\mathbf{s}})^T H(\mathbf{s} - \bar{\mathbf{s}}) = \sum_{i,j} (s_i - \bar{s}_i)(s_j - \bar{s}_j) H_{ij} \).

We now introduce the following symbols for the specific growth rate and its first- and second partial derivatives to the trait value, evaluated in the mean trait value:

\[
g = \left. r(\mathbf{s}) \right|_{\mathbf{s} = \bar{\mathbf{s}}}
\]

\[
g_i = \left. \frac{\partial}{\partial s_i} r(\mathbf{s}) \right|_{\mathbf{s} = \bar{\mathbf{s}}}
\]

\[
g_{ij} = \left. \frac{\partial^2}{\partial s_i \partial s_j} r(\mathbf{s}) \right|_{\mathbf{s} = \bar{\mathbf{s}}}
\]

Analogous expressions for higher-order derivatives are straightforward, and will occasionally be used.

Replacing the vector and matrix products in (3.27) by summations:

\[
\frac{\partial}{\partial t} C_T \approx \int c(\mathbf{s}) \left( g + \sum_{j=1}^{S} (s_j - \bar{s}_j) g_j + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} (s_j - \bar{s}_j)(s_k - \bar{s}_k) g_{jk} \right) d\mathbf{s}
\]

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Moving the integral inwards:

\[
\frac{\partial}{\partial t} C_T \approx \int c(s) g ds + \sum_{j=1}^{S} \int (s_j - \bar{s}_j) g_j c(s) ds \\
+ \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} \int (s_j - \bar{s}_j)(s_k - \bar{s}_k) g_{jk} c(s) ds
\]

Since the specific growth rate and its partial derivatives are evaluated in the average trait, these are independent of the integration variable \(s\) and may therefore be moved out of the integrals:

\[
\frac{\partial}{\partial t} C_T \approx g \int c(s) ds + \sum_{j=1}^{S} g_j \int (s_j - \bar{s}_j) c(s) ds + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} \int (s_j - \bar{s}_j)(s_k - \bar{s}_k) c(s) ds 
\]  

(3.28)

We now substitute the total biomass (3.2) and central moments (3.4), reducing (3.28) to

\[
\frac{\partial}{\partial t} C_T \approx C_T \left( g + \sum_{j=1}^{S} g_j M_j + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} M_{jk} \right).
\]

(3.29)

First-order central moments \(M_j\) equal zero, causing the first-order term to drop out. This finally renders the following, relatively simple approximation for the (population dynamics part of) evolution of total biomass:

\[
\frac{\partial}{\partial t} C_T \approx C_T \left( g + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} M_{jk} \right).
\]

(3.30)

We note again that in this approximation the third- and higher order terms in the Taylor series for the specific growth rate are neglected (cf. Norberg et al. 2001; Wirtz and Eckhardt 1996). The first omitted term equals \(\frac{1}{6} C_T \sum_{j=1}^{S} \sum_{k=1}^{S} \sum_{l=1}^{S} g_{jkl} M_{jkl}\), which would be negligible if third-order central moments (the skewness) approach zero and/or the third partial derivatives to the trait value approach zero – Wirtz & Eckhardt (1996) argue the latter is not uncommon.

3.8.2 Mean

For (3.24), the time derivative of the mean of the \(l\)th trait (3.11) equals

\[
\frac{\partial}{\partial t} \bar{s}_l = \frac{1}{C_T} \left( \int s_l r(s) c(s) ds - \bar{s}_l \frac{\partial}{\partial t} C_T \right) = \frac{1}{C_T} \int (\bar{s}_l - \bar{s}_l) r(s) c(s) ds
\]

We now substitute the total biomass (3.2) and central moments (3.4), reducing (3.28) to

\[
\frac{\partial}{\partial t} C_T \approx C_T \left( g + \sum_{j=1}^{S} g_j M_j + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} M_{jk} \right).
\]

(3.29)

First-order central moments \(M_j\) equal zero, causing the first-order term to drop out. This finally renders the following, relatively simple approximation for the (population dynamics part of) evolution of total biomass:

\[
\frac{\partial}{\partial t} C_T \approx C_T \left( g + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} M_{jk} \right).
\]

(3.30)

We note again that in this approximation the third- and higher order terms in the Taylor series for the specific growth rate are neglected (cf. Norberg et al. 2001; Wirtz and Eckhardt 1996). The first omitted term equals \(\frac{1}{6} C_T \sum_{j=1}^{S} \sum_{k=1}^{S} \sum_{l=1}^{S} g_{jkl} M_{jkl}\), which would be negligible if third-order central moments (the skewness) approach zero and/or the third partial derivatives to the trait value approach zero – Wirtz & Eckhardt (1996) argue the latter is not uncommon.
Replacing the specific growth rate $r(s)$ by its Taylor series about the average trait (3.26)

$$\frac{\partial}{\partial t} \bar{s}_i = \frac{1}{C_T} \int (s_i - \bar{s}_i) \left( \sum_{i=0}^{\infty} \frac{1}{i!} \left[ \sum_{j=1}^{s} (s_j - \bar{s}_j) \frac{\partial}{\partial s_j} r(s) \right] \right) c(s) ds$$

If we neglect third- and higher order terms in the Taylor series, we obtain

$$\frac{\partial}{\partial t} \bar{s}_i \approx \frac{1}{C_T} \int \left( (s_i - \bar{s}_i) g + \sum_{j=1}^{s} (s_i - \bar{s}_i) (s_j - \bar{s}_j) g_j + \frac{1}{2} \sum_{j=1}^{s} \sum_{k=1}^{s} (s_i - \bar{s}_i) (s_j - \bar{s}_j) (s_k - \bar{s}_k) g_{jk} \right) c(s) ds$$

Rearranging integrals and derivatives:

$$\frac{\partial}{\partial t} \bar{s}_i \approx \frac{1}{C_T} g \int (s_i - \bar{s}_i) c(s) ds + \frac{1}{C_T} \sum_{j=1}^{s} g_j \int (s_i - \bar{s}_i) (s_j - \bar{s}_j) c(s) ds + \frac{1}{2} \frac{1}{C_T} \sum_{j=1}^{s} \sum_{k=1}^{s} g_{jk} \int (s_i - \bar{s}_i) (s_j - \bar{s}_j) (s_k - \bar{s}_k) c(s) ds$$

All integrals correspond to central moments of the biomass distribution, allowing us to simplify the above to

$$\frac{\partial}{\partial t} \bar{s}_i \approx g M_i + \sum_{j=1}^{s} g_j M_{ij} + \frac{1}{2} \sum_{j=1}^{s} \sum_{k=1}^{s} g_{jk} M_{jkl}$$

Since $M_i = 0$, the first term drops out, and we finally obtain for the evolution of the mean:

$$\frac{\partial}{\partial t} \bar{s}_i \approx \sum_{j=1}^{s} g_j M_{ij} + \frac{1}{2} \sum_{j=1}^{s} \sum_{k=1}^{s} g_{jk} M_{jkl}.$$  \hspace{1em} (3.31)

For the one-trait case $l = S = 1$, this reduces to the result of Norberg et al. (2001). Retracing our steps, we can with relative ease determine that the first omitted (third-order) term in the above equals $\frac{3}{2} \sum_{j=1}^{s} \sum_{k=1}^{s} \sum_{m=1}^{s} g_{jkm} M_{jkm}$. 

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3.8.3 Covariances

For second-order central moments $C_r M_{lm}$ of the biomass distribution, the population dynamics component of its evolution is given by

$$\frac{\partial}{\partial t} (C_r M_{lm}) = \frac{\partial}{\partial t} \int r(s) c(s) (s_l - \bar{s}_l) (s_m - \bar{s}_m) ds$$

Moving the derivative to time inward and repeatedly applying the product rule for differentiation:

$$\frac{\partial}{\partial t} (C_r M_{lm}) = \int r(s) c(s) (s_l - \bar{s}_l) (s_m - \bar{s}_m) ds$$

By moving the time derivatives of the mean (which are independent of $s$) out of last two integrals, one may recognize in these last terms the product of the derivative of a mean and a first-order central moment. As first-order central moments equal zero, the last two terms simply disappear, leaving us with

$$\frac{\partial}{\partial t} (C_r M_{lm}) = \int r(s) c(s) (s_l - \bar{s}_l) (s_m - \bar{s}_m) ds$$

Replacing the specific growth rate $r(s)$ by its Taylor series about the average trait (3.26)

$$\frac{\partial}{\partial t} (C_r M_{lm}) = \int \left( \sum_{i=0}^{m} \sum_{j=1}^{s} (s_j - \bar{s}_j) \frac{\partial}{\partial s_j} r(s) |_{s=s} \right) c(s) (s_l - \bar{s}_l) (s_m - \bar{s}_m) ds$$

Neglecting third- and higher order terms in the Taylor series, one obtains the approximation

$$\frac{\partial}{\partial t} (C_r M_{lm}) \approx \int \left( \frac{1}{2} \sum_{j=1}^{s} (s_j - \bar{s}_j)^2 g_j + \sum_{j=1}^{s} (s_j - \bar{s}_j) g_j \right) (s_l - \bar{s}_l) (s_m - \bar{s}_m) c(s) ds$$
3.9 Moment closure for population growth

Rearranging integrals and derivatives, and substituting moments when possible:

\[
\frac{\partial}{\partial t}(C_T M_{lm}) \approx C_T \left(g M_{lm} + \sum_{j=1}^{S} g_j M_{jlm} + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} M_{jklm}\right).
\]  

(3.32)

in which the first omitted term equals \(\frac{1}{6} \sum_{j=1}^{S} \sum_{k=1}^{S} \sum_{n=1}^{S} g_{jkn} M_{jknlm}\).

By the quotient rule, we have

\[
\frac{\partial}{\partial t} M_{lm} = \frac{\frac{\partial}{\partial t} (C_T M_{lm})}{C_T} - M_{lm} \frac{\partial}{\partial t} C_T.
\]

Combining this with the approximation of \(\frac{\partial}{\partial t} C_T\) given by (3.30), we have

\[
\frac{\partial}{\partial t} M_{lm} \approx \sum_{j=1}^{S} g_j M_{jlm} + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} \left(M_{jklm} - M_{jkm} M_{lm}\right)
\]

(3.33)

which for the one-trait case \(l = m = S = 1\) simplifies to the variance dynamics derived by Norberg et al. (2001). Again, we can retrace our steps to find the first neglected (third-order) term equals \(\frac{1}{6} \sum_{j=1}^{S} \sum_{k=1}^{S} \sum_{n=1}^{S} g_{jkn} M_{jknlm}\); this in fact combines the first neglected term in (3.30) and the first neglected term in (3.32).

3.9 Moment closure for population growth

In the approximated dynamics of the biomass, mean and variance as given by (3.30), (3.31) and (3.33), higher-order moments of the trait value distribution appear. Specifically, they depend on the third and fourth-order central moments. While one can derive equations for the dynamics of these higher-order moments using the same technique as above, this solves little, as in those equations central moments of even higher order would appear. This is known as the moment closure problem: one has to make certain assumptions to cut-off the infinite moment series at a certain point.

Different approaches for moment closure exist. In turbulence modelling, higher-order moments are typically approximated by functions of lower-order moments, with coefficients in these functions determined by empirical data (e.g., Burchard et al. 1999). Norberg et al. (2001) follow a similar approach, by expressing the third- and fourth-order moments of their (univariate) trait distribution in terms of first- and second-order moments, and estimating parameters for these expressions from simulations with a discretized trait distribution. Wirtz & Eckhardt (1996) take a different route, by directly assuming that their (univariate) trait distribution approximates the normal distribution. Then, even higher-order (>2) central moments can be expressed in terms of the second-order central moment (variance), whereas odd central moments all equal zero.

We consider the amount of empirical data available on natural trait distributions insufficient for derivation of (empirical) moment closure approximations for trait-based ecosystem models. The main reason for this is that such a moment closure would require quantitative knowledge on both the trait values and abundances of a substantial sample of natural species. Such information is in limited supply, and typically too sparse for accurate estimation of distributional moments, in particular
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when it comes to (potentially multivariate) high-order moments such as skewness and kurtosis.

The alternative approach of Norberg et al. (2001), i.e., deriving moment closure coefficients form the results of brute-force simulations with a discretized trait distribution, is attractive but requires a large computational effort; also, this effort increases exponentially with the number of traits. Simulations with discretized univariate trait distributions are feasible (Norberg et al. 2001), as are simulations with discretized bivariate distributions (chapter 2), but with more traits one rapidly reaches the limits of computational resources. Additionally, there is no guarantee that parameterizations for higher-order moments derived from results of discretized reference simulations apply equally well under different environmental conditions: guaranteed accurate closure expressions would require simulations with discretized distribution in all environments of interest, but this is not feasible, and would take away the need for a moment-based approach in the first place.

Therefore, we aim for a moment closure that does not require empirical information on trait distributions, nor discretization of trait distributions. Inspired by the work of Wirtz & Eckhardt (1996), we derive a moment closure by assuming a particular shape for the distribution. First, we follow Wirtz & Eckhardt in assuming the shape of a normal distribution. Second, we expand on this by assuming a normal distribution of the log-transformed traits, i.e. a log-normal distribution of the traits themselves.

3.9.1 Normal distribution

Let us assume that the trait value distribution is well approximated by a multivariate normal distribution, i.e.

\[ c(s) \approx \frac{C_T}{(2\pi)^{\frac{2\lambda}{2}} \sqrt{\det \Sigma}} e^{-\frac{1}{2}(s - \bar{s})^T \Sigma^{-1} (s - \bar{s})}, \]

in which \( \Sigma \) denotes the covariance matrix of \( s \) with \( \Sigma_{ij} = E[(s_i - \bar{s}_i)(s_j - \bar{s}_j)] = M_{ij} \), and \( \det \Sigma \) denotes the determinant of the covariance matrix. For this distribution, all odd central moments equal zero, whereas even moments of order > 2 can be expressed in terms of the second-order central moments (Le Bellac 1995). For a \( k \)th order moments with \( k = 2\lambda \):

\[ M_{c_1 \ldots c_{2\lambda}} = \sum M_{c_1 c_2} M_{c_3 c_4} \ldots M_{c_{2\lambda-1} c_{2\lambda}} \]

with the sum taken over all permutations of \( \{1, \ldots, 2\lambda\} \), rendering \( (2\lambda - 1)! / (2^{\lambda-1}(\lambda - 1)! \) terms. This implies for the fourth-order central moments:

\[ M_{jklm} = M_{jk} M_{lm} + M_{jl} M_{km} + M_{jm} M_{kl} \]

(3.34)
Given that the third-order central moments equal zero, and that the fourth-order central moments are given by (3.34), the dynamics of the trait distribution as defined by (3.30), (3.31) and (3.33) reduce to:

\[
\frac{\partial}{\partial t} C_T \approx C_T \left( g + \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} M_{jk} \right) \\
\frac{\partial}{\partial t} \tilde{s}_i \approx \sum_{j=1}^{S} g_{ji} M_{ji} \\
\frac{\partial}{\partial t} M_{lm} \approx \frac{1}{2} \sum_{j=1}^{S} \sum_{k=1}^{S} g_{jk} \left( M_{jm} M_{km} + M_{jm} M_{kl} \right)
\]  

(3.35)

Under certain simplifying assumptions, we can recognize in this system results of other studies: for two traits (\(S = 2\)), the dynamics of the mean equal those described by Abrams et al. (1993, appendix 2), for a multivariate trait distribution that arises through mutation the dynamics of the mean equal those described by Dieckmann & Law (1996, eq. 6.1), and for a single trait (\(S = 1\)) the dynamics of the mean and variance equal those in Wirtz & Eckhardt (1996).

Many biological traits represent non-negative quantities, e.g. investment in defence, individual size, or the capacity for resource harvesting. The distribution of these quantities can never be truly normal, as that would imply a feasible range from \(-\infty\) to \(\infty\). In practice, this does not need to be a problem, as the trait value distribution might simply be close to normal with the far majority of biomass positioned at positive trait values. However, our simulations have shown (results unpublished) that for (3.35) the mean and/or variance can drift to negative, thus unrealistic values; this behaviour appears to be independent of the accuracy of numerical schemes used, and must therefore indicate a characteristic of the analytical solution of (3.35). This is also easily seen in (3.35): \(\frac{\partial}{\partial t} \tilde{s}_i\) and \(\frac{\partial}{\partial t} M_{lm}\) can be negative even if \(\tilde{s}_i\) and \(M_{lm}\) equal zero, respectively, thus allowing the mean and variance to achieve negative values [this in fact depends on the value of \(g_j\) and \(g_{jk}\), but there is no guarantee that these partial derivative are indeed zero at the boundaries of the feasible trait range]. The occurrence of negative mean and/or variance for positive definite traits is typically unwanted, first because it causes a qualitative departure from the true solution (3.1), and second because the behaviour of the specific growth rate and its derivatives is not defined for negative trait values, and therefore cannot be evaluated at negative mean.

To overcome these problems, we develop another moment closure under the assumption that traits are log-normally distributed (Keeling 2000), and therefore always positive.

### 3.9.2 Log-normal distribution

Let us now assume that the trait value distribution is well approximated by a multivariate log-normal distribution, i.e.

\[
c(s) \approx \frac{C_T}{(2\pi)^{S/2} \sqrt{\det \Sigma} \prod_{i=1}^{S} \tilde{s}_i} e^{-\frac{1}{2} (\ln s - \tilde{s})^T \Sigma^{-1} (\ln s - \tilde{s})}
\]

(3.36)
in which \( \bar{s} \) denotes the mean of \( \ln s \), \( \Sigma \) denotes the covariance matrix of \( \ln s \) with \( \Sigma_{ij} = \mathbb{E}[(\ln s_i - \bar{s}_i)(\ln s_j - \bar{s}_j)] \), and \( \det \Sigma \) denotes the determinant of the covariance matrix.

By definition, the natural logarithm of a log-normally distributed variable follows a normal distribution. One can therefore with relative ease apply our moment-based framework and normal-distribution based moment closure (3.35) to log-normally distributed traits by taking the log-transform of those traits: we define log-transformed trait vector \( \bar{s} \) with \( \bar{s}_i = \ln s_i \). The transformed variates then follow normal distribution

\[
\hat{\mathcal{C}}(\bar{s}) \approx \frac{C_T}{(2\pi)^{n/2} \det \Sigma} e^{-\frac{1}{2}(\bar{s} - \bar{s})^T \Sigma^{-1}(\bar{s} - \bar{s})},
\]

This implies that (3.35) can approximate the evolution of the mean and variance of \( \bar{s} \), provided we define the growth rate in terms of \( \bar{s} \), i.e. \( \dot{\bar{s}}(\bar{s}) = r(\bar{s}) \big|_{s = e^\bar{s}} \), and take its first- and second derivative to elements of \( \bar{s} \) instead of \( s \).

One might stop here, satisfied in knowing that (3.35) describes the dynamics of any multivariate log-normal distribution if trait values are log-transformed. However, in some cases this is not sufficient. Through the log-transformation, the system is now completely defined in terms of moments of the log-transformed variables \( \bar{s} \). Transformation of these into moments of the untransformed \( s \) is not trivial, as this is dependent on the shape of underlying distribution. Yet one sometimes takes interest in the moments of the untransformed \( s \). For instance, in chapter 4 a log-normal transformation of traits is applied, but the (untransformed) mean of the traits and its derivative to time still feature explicitly in differential equations for other state variables. We therefore will derive explicit expressions for the mean and (co)variance of log-normally distributed traits.

From the mean and covariances of \( \bar{s} \) one can calculate the mean and covariances of the untransformed \( s \):

\[
\bar{s}_i = e^{\bar{s}_i} + \bar{M}_{ii}/2
\]

\[
M_{ij} = (e^{\bar{M}_{ij}} - 1) e^{\bar{s}_i} + \bar{s}_j + \frac{1}{2}(\bar{M}_{ii} + \bar{M}_{jj}) = (e^{\bar{M}_{ij}} - 1) \bar{s}_i \bar{s}_j
\]

according to Johnson & Kotz (1972). In turn, this gives the raw second-order moments

\[
M'_{ij} = e^{\bar{M}_{ij}} + \bar{s}_i + \bar{s}_j + \frac{1}{2}(\bar{M}_{ii} + \bar{M}_{jj})
\]
From (3.36), we can derive that the time derivatives of the mean and variance of the untransformed $s$ equal

$$
\frac{d}{dt} \tilde{s}_i = \left( \frac{d}{dt} \tilde{s}_i + \frac{1}{2} \frac{d}{dt} \tilde{M}_{ii} \right) \tilde{s}_i
$$

$$
\frac{d}{dt} M_{ij} = \left( \frac{d}{dt} \tilde{M}_{ij} + \frac{1}{2} \frac{d}{dt} \tilde{s}_i + \frac{1}{2} \frac{d}{dt} \tilde{s}_j + \frac{1}{2} \frac{d}{dt} \tilde{M}_{ii} + \frac{1}{2} \frac{d}{dt} \tilde{M}_{jj} \right) \left( M_{ij} + \tilde{s}_i \tilde{s}_j \right)
$$

in which differential equations for the moments of the transformed $\tilde{s}$, i.e. $d\tilde{M}_{ij}/dt$ and $d\tilde{M}_{ij}/dt$ are given by (3.35) applied to the transformed moments and growth rate. The moments of the transformed $\tilde{s}$ that then appear in the result can be calculated from the moments of the untransformed $s$:

$$
\tilde{s}_i = \ln \frac{\tilde{s}_i}{\sqrt{\tilde{M}_{ii}/\tilde{s}_i^2 + 1}} = \ln \frac{\tilde{s}_i^2}{\sqrt{\tilde{M}_{ii}}}
$$

$$
\tilde{M}_{ij} = \ln \left( \frac{M_{ij}}{\tilde{s}_i \tilde{s}_j} + 1 \right) = \ln \frac{M_{ij}^2}{\tilde{s}_i \tilde{s}_j}
$$

which directly follows from (3.36).

### 3.10 References


3. An approximation for succession-based dynamics of trait distributions


4  An adapting ecosystem manoeuvring between autotrophy and heterotrophy

Submitted manuscript

Abstract
The functioning of ecosystems is a direct consequence of the structure and diversity of the species community, which can be difficult to represent in models. Complex Adaptive System (CAS) theory perceives the community as a single adapting entity, and features concepts that can help to incorporate community structure in models without introducing great complexity. In this study a CAS-type approach, adapted to accommodate spatial structure, is used to describe spatiotemporal variation in the structure of plankton communities. A diverse community of phytoplankton and bacteria is represented by an evolving distribution of autotrophy and heterotrophy. Embedded in a vertically structured model of a water column and exposed to realistically varying environmental conditions, the model reproduces several trends well-known from the aquatic literature, e.g., seasonal succession with autotrophic species being replaced by mixotrophs and heterotrophs, and the formation of a shade flora and a deep chlorophyll maximum. Such qualitative agreements with observations suggest that trait-based adaptive ecosystem models are capable of elegant, simple parameterizations that preserve key ecosystem behaviours, and as such can contribute to the insight in community assembly.
4. An adapting ecosystem manoeuvring between autotrophy and heterotrophy

4.1 Introduction
The functioning of ecosystems is a direct consequence of the structure and diversity of the species community (Loreau et al. 2001). Therefore, understanding and predicting many ecosystem phenomena requires a view that goes beyond the traditional distinction of a few functional groups, and provides insight into the community structure and the process of community assembly. However, resolution of the structure and assembly of communities in food web models is not a trivial task. Community models are often constructed by combining population models of multiple species, with related species represented by the same model with different parameter sets. For instance, phytoplankton community models often use one model structure, with species differing in traits such as nutrient affinity, maximum growth rate, mortality, sinking rate, palatability and light affinity (Evans 1988; Lancelot et al. 2005; Merico et al. 2004; Reynolds et al. 2001). The resulting aggregate models produce straightforward results, but tend to suffer from underdetermination of parameter values and the inevitable necessity of limiting the model to a subset of all actual species (Anderson 2005; Bruggeman and Kooijman 2007): arguably, these models are simultaneously too complex and too simple.

Recently, promise was shown by approaches that incorporate principles from frameworks for adaptation (Abrams et al. 1993), evolutionary biology (Dieckmann and Law 1996) and quantitative genetics (Norberg et al. 2001) to produce elegant parameterizations of community behaviour. In the spirit of Complex Adaptive Systems (CAS) theory (Holland 1996; Levin 1998), these approaches perceive the community or ecosystem as single entity, adapting in response to internal and environmental pressures. This entity is modelled as a continuum of different species, all represented by the same, unified population model and differing only in the value of a few key traits subject to trade-offs. Not individual species, but aggregate variables such as the total community biomass and trait means are then followed in time. For instance, Wirtz and Eckhardt (1996) modelled phytoplankton succession in a lake ecosystem as a shift in the average maximum growth rate of phytoplankton (correlated with nutrient half-saturation and edibility to produce a trade-off) and the fraction of diatoms in the community. Jiang et al. (2005) demonstrated the evolution of a community of phytoplankton and zooplankton by modelling the dynamics of the average size of each group. Similar principles were used in chapter 2 to model phytoplankton succession as a shift in light- and nutrient harvesting investments within the community.

The applicability of CAS-type approaches is not limited to the theoretical studies where they are often found (Norberg et al. 2001; Savage et al. 2007), and they can incorporate features such as spatial structure and temporally variable forcing with relative ease. In the present study we demonstrate a CAS-type approach that resolves the well-known pattern of seasonal, depth-dependent assembly of a plankton...
4.2 Modelling approach

4.2.1 The generic population

The validity of trait-based community models depends on the extent to which the selected traits can explain the outcome of interspecific competition. Plankton succession is often discussed in terms of bottom-up versus top-down control: succession of species is said to be governed by lower trophic levels, e.g., through nutrient limitation (Margalef 1978; Tilman 1977; Tilman 1981; Tilman 1982) or higher trophic levels, e.g., through predation (Carpenter and Kitchell 1993; Porter 1973). Much less explored is the more recent idea that plankton community assembly can be linked to mixotrophy: the capability of species to utilize organic as well as inorganic substrates (Cloern and Dufford 2005; Smayda 1997). This is a widespread phenomenon in aquatic systems (Kooijman and Hengeveld 2005): numerous plankton species combine a heterotrophic feeding mode (e.g., extracellular digestion,
phagotrophy) with an autotrophic one: “autotrophy and heterotrophy ... are two extremes of a continuum of strategies” (Dolan and Perez 2000). Mixotrophy has been suggested to play a defining role in succession of plankton species: the textbook phytoplankton successional sequence describes a shift from mostly autotrophic species (diatoms) to mixotrophic and heterotrophic species (dinoflagellates) over spring and summer (Chang et al. 2003), which is often difficult to capture in terms of bottom-up and top-down controls. In this study we explore to what extent shifts in the balance between autotrophy and heterotrophy can explain species succession in plankton communities.

To represent populations with arbitrary levels of autotrophic and heterotrophic activity, we develop a unified model that features an autotrophic route (i.e., photosynthesis) as well as a heterotrophic route (e.g., phagotrophy, extracellular digestion). In the former light and nutrient are combined to form new biomass, and in the latter organic matter is converted into new biomass. This representation of mixotrophy is conceptually similar to previous work (Kooijman et al. 2002; Troost et al. 2005a), but here we rigorously minimize physiological detail to focus instead on energy-based trade-offs associated with the different assimilation routes. Newly synthesized biomass is partitioned over three pools: (1) autotrophic biomass, i.e., chlorophyll and associated machinery (Geider et al. 1996; Klausmeier et al. 2004), (2) heterotrophic biomass, i.e., machinery for heterotrophic activity (Hansen et al. 2000; Raven 1997), and (3) structural biomass (Bruggeman and Kooijman 2007). For the sake of simplicity the stoichiometry of the three types of biomass is taken equal; they are also expressed in the same unit. Structural biomass is denoted by $V$. The partitioning of biomass across the three pools is quantified by species-specific partition coefficients $m_L$ and $m_H$, which denote the allocation (of energy and mass) to autotrophy and heterotrophy, respectively, relative to the allocation to structural biomass. Differences between species can be accounted for by differences in the allocation coefficients; by varying these coefficients we can span the entire range from pure autotrophs ($m_L > 0, m_H = 0$), via mixotrophs ($m_L > 0, m_H > 0$), to pure heterotrophs ($m_L = 0, m_H > 0$), and additionally distinguish high-chlorophyll and low-chlorophyll species (high $m_L$ vs. low $m_L$).

In photosynthesis light $X_L$ and nutrient $X_N$ are combined to form new biomass. We assume that the effective availability of light is proportional to the amount of autotrophic biomass, and model the photosynthesis reaction with a 2-substrate synthesizing unit (Kooijman 1998; Kooijman 2000; Muller et al. 2001). The structure-specific rate at which new biomass is produced in photosynthesis is then given by

$$j_{AA} = \frac{j_{AM,A}}{1 + \frac{K_L}{m_L X_L} \left( \frac{m_L X_L}{K_N} \right)^{m_H}},$$

in which $j_{AM,A}$ denotes the maximum structure-specific rate of biomass production by autotrophy, $K_L$ denotes the half-saturation light intensity at $m_L = 1$, and $K_N$ denotes the half-saturation nutrient concentration (Bruggeman and Kooijman 2007). The
above is equivalent to a Holling type II functional response, extended to use two complementary resources (Kooi et al. 2004).

Simultaneously, biomass is produced via the heterotrophic route according to a Holling type II functional response

\[
 j_{A,H} = \frac{j_{Am,H}}{1 + m_D K_D}
 \]

(4.2)

in which \( j_{Am,H} \) denotes the maximum structure-specific rate of biomass production by heterotrophy and \( K_D \) the half-saturation organic matter concentration at \( m_D = 1 \).

Biomass produced along the autotrophic and heterotrophic routes is partitioned over structural biomass, autotrophic machinery and heterotrophic machinery, according to species-specific coefficients \( m_L \) and \( m_P \). Thus the specific rate at which new structural biomass is formed is given by

\[
 j_{VA,AA} = \frac{j_{AA}}{1 + m_L + m_D}
 \]

\[
 j_{VA,H} = \frac{j_{AH}}{1 + m_L + m_D} ,
 \]

(4.3)

for the autotrophic and heterotrophic routes respectively.

All biomass is assumed to require maintenance, i.e., a fixed amount of energy per unit time. The maintenance requirement is taken to be fulfilled by mobilization (i.e., breakdown) of structural biomass; the mobilized energy fuels maintenance, while mass leaves the cell as mineral compounds that contribute to the external nutrient pool.

Energy fixed in assimilation machinery cannot be remobilized; harvesting machinery decays passively with structural biomass. Given these assumptions, the specific rate at which structural biomass is mobilized for maintenance equals

\[
 j_{VM} = (1 + m_L + m_D) j_M ,
 \]

(4.4)

in which \( j_M \) denotes the constant maintenance requirement (in structural biomass units) per unit of biomass. Finally, we impose a constant mortality \( j_H \) which transforms living biomass into dead organic matter; this organic matter will in turn be available to the heterotrophic assimilation machinery.

We now collect autotrophic and heterotrophic terms that affect structural biomass:

\[
 r_A = j_{VA,AA} - j_{VM} = \frac{j_{AA}(m_L)}{1 + m_L + m_D} - (1 + m_L + m_D) j_M
 \]

\[
 r_H = j_{VA,H} - j_H = \frac{j_{AH}(m_D)}{1 + m_L + m_D} - j_H
 \]
with \( r_A \) describing the net rate of conversion from nutrient to structural biomass and \( r_H \) describing the net rate of conversion from external organic matter to structural biomass. The specific growth rate of structural biomass becomes

\[
r = r_A + r_H = \frac{j_A A(m_L) + j_A H(m_D)}{1 + m_L + m_D} - (1 + m_L + m_D)j_M - j_H. \tag{4.5}
\]

The dynamic behaviour of the nutrient, organic matter, structural biomass system is now given by

\[
\begin{align*}
\frac{d}{dt} X_N & = -(1 + m_L + m_D)V r_A \\
\frac{d}{dt} X_H & = -(1 + m_L + m_D)V r_H. \\
\frac{d}{dt} V & = VR \tag{4.6}
\end{align*}
\]

The dynamics of harvesting biomasses are implicitly specified by the dynamics of structural biomass and the species-specific allocation coefficients \( m_L \) and \( m_D \), i.e., \( m_L \frac{dV}{dt} \) and \( m_D \frac{dV}{dt} \) for autotrophic and heterotrophic biomass respectively, and are therefore not explicitly included. Taking this into consideration, the system is clearly closed for mass: \( d\left( (1 + m_L + m_D)V + X_N + X_H \right)/dt = 0 \).

### 4.2.2 Extension to communities

Building upon the unified population model, we now assume that the functional diversity in the community – that is, the diversity that affects aggregate mass- and energy fluxes or the outcome of interspecific competition – can be characterized by a probability distribution of parameters. For the plankton model we select two parameters that are allowed to vary across species: the allocation to autotrophy \( m_L \) and allocation to heterotrophy \( m_D \). The value of the resulting bivariate distribution may be interpreted as the probability of finding a species with given \( (m_L, m_D) \). Model (4.6) is now applied to all ecosystem species. Differential growth and mortality of species translates into evolution of the trait distribution, in the form of relative increases in biomass at (temporally and spatially) local fitness optima: the trait value combinations with the highest net specific growth rate. Coefficients \( m_L \) and \( m_D \) are subject to trade-offs: while higher values increase the affinity for the corresponding resource (eqns. 1 and 2), they also increase the costs for growth of structural biomass (eqn. 3) and maintenance (eqn. 4). These effects are a direct result of the partitioning of assimilated energy and matter over the different metabolic activities, and correspond to trade-offs commonly associated with the use of additional assimilation routes: mixotrophs are thought to incur higher costs for synthesis of assimilation machinery and to have higher respiration (maintenance) rates (Raven 1997; Rothhaupt 1996; Stoecker 1998). In view of this correspondence with observations, the present model compares favourably with previous models that assumed more ad-hoc trade-offs for mixotrophy (Thingstad et al. 1996; Troost et al. 2005a). On a more detailed level, one can observe that the present trade-offs between resource affinity and net growth constrain the trait distribution: the benefit at increasing trait values
saturates whereas costs for growth and maintenance increase linearly; this implies that very high trait values are non-viable, and thus provides an upper boundary for the trait value.

One means of modelling the dynamics of the trait distribution is to discretize the trait dimensions and model the fate of the mass within each trait interval explicitly (Bruggeman and Kooijman 2007); this allows for arbitrary accuracy (by modifying grid size) and flexibility in distribution shape, but it is computationally expensive. Alternatively, one can characterize the distribution by one or more key statistics and model their dynamics. Here, an intuitive option is to focus on the moments of the trait distribution, i.e., the total biomass, the mean trait values, and trait covariances.

4.2.3 Approximate dynamics of trait distribution moments

For any population model that (1) includes community diversity through a probability distribution imposed on one or more traits and (2) assumes the trait-dependent part of population growth is proportional to structural population biomass, one can derive expressions for the dynamics of the distributional moments (Norberg et al. 2001; Savage et al. 2007). First we define trait distribution as the product of the probability distribution of trait values (its integral over trait space equal to one) and the total structural biomass in the community. This distribution is obviously time-dependent, but for the sake of readability we suppress this dependency in the following derivation. For the mixotrophic community, the total structural biomass can now be written as

\[ V_T = \int \int v(m_L, m_D) dm_L dm_D. \]

The dynamic behaviour of a single species in trait space, i.e., \( dv(m_L, m_D)/dt \) is now prescribed by \( dV/dt \) in (4.6), with \( V \) replaced by \( v(m_L, m_D) \). The dynamic behavior of the total structural biomass is thus given by

\[ \frac{d}{dt} V_T = \frac{d}{dt} \int \int v(m_L, m_D) dm_L dm_D = \int \int v(m_L, m_D)r(m_L, m_D) dm_L dm_D, \quad (4.7) \]

with \( r(m_L, m_D) \) denoting the specific growth rate (4.5). We now Taylor expand the specific growth rate around the distributional mean \( (\mu_L, \mu_D) \):

\[
r(m_L, m_D) = r|_{m_L=\mu_L, m_D=\mu_D} + (m_L - \mu_L)g_b + (m_D - \mu_D)g_d + \frac{1}{2}(m_L - \mu_L)^2 h_{1b} + (m_L - \mu_L)(m_D - \mu_D)h_{1d} + \frac{1}{2}(m_D - \mu_D)^2 h_{2d} + \ldots,
\]

with \( g_i \) denoting the first derivative of \( r \) to trait \( m_i \) evaluated at the mean, and every \( h_{ij} \) denoting a second derivative of \( r \) to \( m_i \) and \( m_j \) evaluated at the mean:
Substituting the Taylor expansion in (4.7), rearranging, and substituting the first and second central moments defined by

\[ 0 = \frac{1}{v} \int \sum \rightarrow \int (m_i - \mu_i) \nu(m_L, m_D) \, dm_L \, dm_D \]

\[ \sigma_{ij} = \frac{1}{v} \int \left( \sum \right) (m_i - \mu_i)(m_j - \mu_j) \nu(m_L, m_D) \, dm_L \, dm_D \]

we obtain

\[ \frac{d}{dt} V_r = V_r \left( \right) \frac{1}{v} \int \left( \right) \sigma_{LL} h_{LL} + \sigma_{LD} h_{LD} + \frac{1}{2} \sigma_{DD} h_{DD} + \ldots \)

in which \( \sigma_{LL} \) denotes the variance of \( m_L \), \( \sigma_{LD} \) the covariance of \( m_L \) and \( m_D \), and \( \sigma_{DD} \) the variance of \( m_D \). In this expression the omitted higher-order terms contain the higher-order central moments (skewness, kurtosis, etc.). Thus, the dynamics of the total structural biomass are given by an infinite series of terms that combine derivatives of the specific growth rate to the traits, and central moments of the trait distribution. Similar expressions can be derived for the dynamics of the mean and the central moments of the distribution (chapter 3).

The infinite series that describe the dynamics of community-integrated variables can be substantially simplified – and are often still well approximated – by neglecting higher-order derivatives of the specific growth rate and introducing moment closures: parameterizations of higher moments (e.g., skewness, kurtosis) in terms of lower moments (mean and covariance). This principle features prominently in frameworks for the modelling of adaptation and evolution (Abrams et al. 1993; Dieckmann and Law 1996; Jiang et al. 2005), and more recently in models for species succession (Norberg et al. 2001; Shipley et al. 2006; Wirtz and Eckhardt 1996), with roots that can often be traced back to theory from quantitative genetics (Waxman and Gavrilets 2005). The exact approximations employed vary. For instance, Abrams et al. (1993) neglect all but the first-order term in the above Taylor expansion to study adaptation-induced changes in the trait mean. Similarly, Dieckmann and Law (1996) describe the dynamics of traits on evolutionary time scales with the first-order term only, although an equation for the mean including higher-order terms is presented. Approximations that omit second- and higher-order terms work particularly well if the trait distribution is symmetrical; then the second-order term, which is proportional to the skewness, equals zero. This is illustrated by Wirtz and Eckhardt (1996), who model the evolution of the mean traits of a plankton community with the first-order term only, motivating this with the assumption that the trait distribution is near-normal. In
contrast, Norberg et al. (2001) take higher-order terms into account to study species succession, and parameterize higher moments using simulation results; this renders accurate approximations but requires information on the behaviour of the full system.

For the present case, we assume that the distribution of autotrophy and heterotrophy is well-approximated by a bivariate log-normal distribution. This allows the use of the simplifications made possible by the normal distribution while simultaneously accounting for the fact that allocation coefficients are non-negative. Assuming a log-normal trait distribution, we obtain straightforward expressions for the evolution of the population biomass and trait means, as well as trait covariances (chapter 3). Key in the derivation is the rephrasing of the system in terms of log-transformed traits: as the trait distribution is assumed to be lognormal, the distribution of log-transformed traits is normal and the simplifications developed for the normal distribution apply. Transformed traits will be denoted with a hat symbol superposed, i.e., $\hat{m}_L = \ln m_L$, $\hat{m}_D = \ln m_D$, and similar notation will be used for moments of the transformed traits, e.g., $\mu_L$ for the mean of $\hat{m}_L$.

Assuming (log-transformed) traits $\hat{m}_L$ and $\hat{m}_D$ have a bivariate normal distribution, the dynamics of the total structural biomass of the community are approximated by

$$\frac{d}{dt} V_T \approx V_T(\hat{\mu}_{\hat{m}_L = \hat{m}_L, \hat{m}_D = \hat{m}_D}) + \frac{1}{2} \sigma_{LL} \hat{h}_{LL} + \sigma_{LD} \hat{h}_{LD} + \frac{1}{2} \sigma_{DD} \hat{h}_{DD},$$

(4.8)

with $\hat{\mu}$ denoting the specific growth rate of the population expressed in the log-transformed traits, each $\sigma_{ij}$ denoting the covariance for traits $\hat{m}_i$ and $\hat{m}_j$ within the community and every $\hat{h}_{ij}$ denoting a second derivative of $\hat{\mu}$ to traits $\hat{m}_i$ and $\hat{m}_j$, evaluated at the mean:

$$\hat{h}_{ij} = \left. \frac{\partial^2 \hat{\mu}}{\partial m_i \partial m_j} \right|_{\hat{m}_L = \hat{m}_L, \hat{m}_D = \hat{m}_D} \text{ for } i, j = L, D.$$

Note that the specific growth rate and its derivatives depend on traits $\hat{m}_L$, $\hat{m}_D$, and environmental variables $X_L$, $X_N$, and $X_D$; these dependencies are suppressed for the sake of readability. The dynamics of the mean of the log-transformed traits can then be approximated by

$$\frac{d}{dt} \hat{\mu}_L \approx \sigma_{LL} \hat{g}_L + \sigma_{LD} \hat{g}_D,$$

$$\frac{d}{dt} \hat{\mu}_D \approx \sigma_{DD} \hat{g}_D + \sigma_{LD} \hat{g}_L,$$

(4.9)

with $\hat{g}_i$ denoting the first derivative of $\hat{\mu}$ to trait $\hat{m}_i$ evaluated at the mean, i.e.,

$$\hat{g}_i = \left. \frac{\partial \hat{\mu}}{\partial m_i} \right|_{\hat{m}_L = \hat{m}_L, \hat{m}_D = \hat{m}_D} \text{ for } i, j = L, D.$$
4. An adapting ecosystem manoeuvring between autotrophy and heterotrophy

The dynamics of the covariances are approximated by

\[
\frac{d}{dt} \sigma_{LL} = \sigma_{LL}^2 \dot{h}_{LL} + \sigma_{LL} \sigma_{LD} (\dot{h}_{LD} + \dot{h}_{DL}) + \sigma_{LD}^2 \dot{h}_{DD} \\
\frac{d}{dt} \sigma_{DD} = \sigma_{DD}^2 \dot{h}_{DD} + \sigma_{DD} \sigma_{LD} (\dot{h}_{LD} + \dot{h}_{DL}) + \sigma_{LD}^2 \dot{h}_{LL} \\
\frac{d}{dt} \sigma_{LD} = \sigma_{LL} \sigma_{LD} \dot{h}_{LL} + \frac{1}{2} (\sigma_{LL} \sigma_{DD} + \sigma_{LD}^2) (\dot{h}_{LD} + \dot{h}_{DL}) + \sigma_{DD} \sigma_{LD} \dot{h}_{DD}
\]

(4.10)

We stress that this is a general result: approximations (4.8), (4.9) and (4.10) apply to any two-trait population model, provided the distribution of traits \( \hat{m}_L \) and \( \hat{m}_D \) is well approximated by a bivariate normal distribution. Analog equations for arbitrary numbers of traits are provided in chapter 3.

With the dynamics of distributional moments completely specified, it remains to find expressions for the behaviour of the nutrient and organic matter. As for the total structural biomass, the dynamics of these variables are given by the corresponding equations in system (4.6), integrated over the trait distribution, i.e.,

\[
\frac{d}{dt} X_N = - \int \int \{ (1 + m_L + m_D) v(m_L, m_D) r_A(m_L, m_D) dm_L dm_D \} \\
\frac{d}{dt} X_D = - \int \int \{ (1 + m_L + m_D) v(m_L, m_D) r_H(m_L, m_D) dm_L dm_D \}
\]

Taylor-expanding the autotrophic- and heterotrophic components of the growth rate, this can be shown to equal

\[
\frac{d}{dt} X_N = \left[ (1 + \mu_L + \mu_D) \frac{d}{dt} V_T + V_T \frac{d}{dt} \mu_L + V_T \frac{d}{dt} \mu_D \right]_{r=r_A} \\
\frac{d}{dt} X_D = \left[ (1 + \mu_L + \mu_D) \frac{d}{dt} V_T + V_T \frac{d}{dt} \mu_L + V_T \frac{d}{dt} \mu_D \right]_{r=r_H}
\]

(4.11)

in which subscripts \( r = r_A \) and \( r = r_H \) signify that for the change in nutrient \( X_N \) only autotrophic components, and for the change in organic matter \( X_D \) only heterotrophic components of the growth rate are considered. In these expressions the dynamics of the (untransformed) trait mean appear, illustrating that changes in the trait mean affect the environment not only indirectly by changing the behaviour of the community, but also directly because the traits represent biomass. The dynamics of the mean of the untransformed trait are implicitly defined by (4.9) and (4.10) if a log-normal distribution is assumed: from the relationship between the mean of log-normally distributed traits and the mean and variance of the log-transformed trait, one can derive expressions for the relation between (approximated) derivatives of the log-transformed traits and the derivatives of untransformed traits (chapter 3). Inserting this expression in (4.11) suffices to express the dynamics of nutrient and biomass in terms of the moments of the log-transformed trait. This completes the formulation of the model in a spatially homogeneous environment. In summary, the biomass, nutrient and organic matter dynamics are given by (4.8) and (4.11), and the
moment dynamics are given by (4.9) and (4.10), resulting in a 8-dimensional ODE system.

4.2.4 Spatial structure and temporal variability

The structure of natural communities is to a large extent shaped by temporal and spatial variation. This is particularly true for aquatic systems (Tilman 1982, Tilman and Kareiva 1997): in temperate regions, seasonal changes in environmental parameters such as light intensity and nutrient concentration induce succession in plankton communities, with a characteristic spring community of phytoplankton species (e.g., diatoms) being replaced by groups of very different species (e.g., dinoflagellates) over the course of spring and summer (Margalef 1958, Reynolds 1984b, Sommer 1987). Spatial heterogeneity is equally important: the structure of plankton communities varies in depth due to light attenuation (Venrick 1982), as acknowledged in the over a century old concept of the “shade flora” (Sournia 1982b). This situation is complicated by turbulence-induced mixing, which redistributes matter across the water column and varies considerably in intensity in time and space. The ensuing spatiotemporal heterogeneity allows for variation of the dominant community type, and additionally affects community diversity: it can promote coexistence of species and prevent competitive exclusion (Chesson 2000).

To account for the role of spatiotemporal heterogeneity, the plankton community model is embedded in a detailed, 100-layer physical model of a marine turbulent water column (Burchard et al. 2006, Burchard et al. 1999). This model is configured with standard settings (Allen et al. 2004, Bruggeman and Kooijman 2007) to describe the top 500 m of a well-known oligotrophic site near Bermuda, in the period 1989-1993 (Steinberg et al. 2001). The vertical light gradient is resolved explicitly, causing the local light intensity to be a function of the incident light intensity $X_i(t,0)$ and depth $z$:

$$X_i(t,z) = X_i(t,0)e^{-z/z_t}, \quad (4.12)$$

with $z_t$ denoting the extinction depth. The incident light intensity $X_i(t,0)$ is calculated from the Julian day number, time of the day and geographic location according to astronomical formula, and attenuated by a realistically varying cloud cover (Uppala et al. 2005); thus seasonal, diurnal and weather-controlled erratic variation in the incident light intensity is accounted for. In addition, the physical model calculates a temporally variable, depth-dependent turbulent diffusivity $D(t,z)$ from observed meteorological variables (Uppala et al. 2005) and vertical gradients of temperature and salinity (http://bats.bios.edu). This diffusivity directly controls the distribution of matter across the water column. Thus, the environment as experienced by the plankton community is summarized by the time- and depth dependent light intensity and diffusivity, shown in Figure 4.1.
An adapting ecosystem manoeuvring between autotrophy and heterotrophy

Figure 4.1. The physical environment as experienced by the plankton community. Shown respectively: the 10-day mean of the light intensity (a) and the turbulent diffusivity (b), as a function of time and depth over a one-year period.

The incorporation of diffusion in models is straightforward for variables that represent mass or energy, but less so for the mean and covariances of the trait distribution. It is possible to derive transport equations for these moments (chapter 3), but it is often simpler to evolve the first- and second non-normalized raw moments. These variables behave as standard tracers with respect to advection and diffusion, and are therefore easily embedded in any existing advection-diffusion framework, and directly specify the mean and variance. Ultimately we rephrase the system in terms of non-normalized raw moments of the log-transformed traits, i.e., \( \bar{g} \), \( \bar{g}^2 \), and \( \bar{g}^3 \), with diffusion added, the dynamics of each biochemical state variable \( c \) at depth \( z \) are given by

\[
\frac{\partial c(t,z)}{\partial t} = \frac{\partial}{\partial z} \left( D(t,z) \frac{\partial c(t,z)}{\partial z} \right) + f(t,z,\ldots),
\]

with \( c = X_X, X_D, \mu_LV, \mu_DV, (\mu_{LL} + \mu_L^2)V, (\mu_{DD} + \mu_D^2)V, (\mu_{LD} + \mu_L\mu_D)V, \) and \( f(t,z,\ldots) \) denoting the contribution of biological processes prescribed by the community model of eqns. (4.11), (4.8) and – after transformation to raw moments of the biomass distribution – (4.9) and (4.10). The column is closed for matter, which translates into Neumann boundary condition

\[
D(t,z) \frac{\partial c(t,z)}{\partial z} \bigg|_{z = -z_{\text{max}}} = 0,
\]

with \( z_{\text{max}} \) denoting the depth of the water column. The initial concentrations of biological variables are homogeneous across the column; characteristic vertical profiles develop over the first two simulated years. The initial nutrient concentration is chosen to match the average nutrient concentration in the top 500 m of the chosen
4.2 Modelling approach

site; initial biomass and organic matter concentrations are low, resembling a winter situation (table 4.1). The initial distributional moments are chosen such that the initial distribution is centred and spread across the relevant range of the traits; this range was determined iteratively by varying the initial mean and variances, and evaluating the ranges taken by the trait means during simulation.

Table 4.1. Symbols used in the model, excluding locally defined auxiliary variables. Listed respectively: state variables and traits of the population model, moments of the trait-based community, forcing variables provided by the physical model, parameters. Parameter values and initial values for the state variables (denoted with superscript *) are to the best of our knowledge representative for oligotrophic plankton communities.

<table>
<thead>
<tr>
<th>symbol</th>
<th>unit</th>
<th>interpretation</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_N$</td>
<td>mmol N m$^{-3}$</td>
<td>nutrient</td>
<td>1*</td>
</tr>
<tr>
<td>$X_D$</td>
<td>mmol N m$^{-3}$</td>
<td>dead organic matter</td>
<td>0.01*</td>
</tr>
<tr>
<td>$V$</td>
<td>mmol N m$^{-3}$</td>
<td>structural biomass of single species</td>
<td></td>
</tr>
<tr>
<td>$m_L$</td>
<td>-</td>
<td>relative investment in autotrophy</td>
<td></td>
</tr>
<tr>
<td>$m_D$</td>
<td>-</td>
<td>relative investment in heterotrophy</td>
<td></td>
</tr>
<tr>
<td>$V_T$</td>
<td>mmol N m$^{-3}$</td>
<td>community structural biomass</td>
<td>0.01*</td>
</tr>
<tr>
<td>$\mu_i$</td>
<td>-</td>
<td>community mean of $m_i$</td>
<td>0.25*</td>
</tr>
<tr>
<td>$\sigma_{ii}$</td>
<td>-</td>
<td>community variance of $m_i$</td>
<td>0.083*</td>
</tr>
<tr>
<td>$\sigma_{ij}$</td>
<td>-</td>
<td>community covariance for $m_i$ and $m_j$</td>
<td>0*</td>
</tr>
<tr>
<td>$\hat{\mu}_i$</td>
<td>-</td>
<td>community mean of log-transformed $m_i$</td>
<td></td>
</tr>
<tr>
<td>$\hat{\sigma}_{ij}$</td>
<td>-</td>
<td>community covariance for log-transformed $m_i$ and $m_j$</td>
<td></td>
</tr>
<tr>
<td>$X_L$</td>
<td>W m$^{-2}$</td>
<td>light intensity</td>
<td></td>
</tr>
<tr>
<td>$D$</td>
<td>m$^2$ s$^{-1}$</td>
<td>turbulent diffusivity</td>
<td></td>
</tr>
<tr>
<td>$K_L$</td>
<td>W m$^{-2}$</td>
<td>reference half-saturation light intensity</td>
<td>0.2</td>
</tr>
<tr>
<td>$K_N$</td>
<td>mmol N m$^{-3}$</td>
<td>half-saturation nutrient concentration</td>
<td>0.35</td>
</tr>
<tr>
<td>$K_D$</td>
<td>mmol N m$^{-3}$</td>
<td>reference half-saturation dead organic matter concentration</td>
<td>10</td>
</tr>
<tr>
<td>$j_{Am,A}$</td>
<td>d$^{-1}$</td>
<td>maximum rate of autotrophic biomass production</td>
<td>1.5</td>
</tr>
<tr>
<td>$j_{Am,H}$</td>
<td>d$^{-1}$</td>
<td>maximum rate of heterotrophic biomass production</td>
<td>20</td>
</tr>
<tr>
<td>$j_M$</td>
<td>d$^{-1}$</td>
<td>biomass maintenance requirement</td>
<td>0.05</td>
</tr>
<tr>
<td>$j_H$</td>
<td>d$^{-1}$</td>
<td>mortality</td>
<td>0.1</td>
</tr>
<tr>
<td>$z_L$</td>
<td>m</td>
<td>extinction depth</td>
<td>20</td>
</tr>
<tr>
<td>$I$</td>
<td>d$^{-1}$</td>
<td>migration rate</td>
<td>0.086</td>
</tr>
</tbody>
</table>
In line with the System of Infinite Diversity (Bruggeman and Kooijman 2007) we impose a permanent presence of trace amounts of all possible species, mimicked by continuous, slow immigration of all species. The continued reintroduction of species is motivated by the observation that in communities of small species (< 1 mm) a constant background diversity tends to be maintained (Fenchel and Finlay 2004); the immigration mechanism is chosen because aquatic communities are for an important part shaped by immigration (Cloern and Dufford 2005; Leibold and Norberg 2004). A constant chemostat-like through-flow \( I \) at all depths is imposed, with concentrations of biochemical variables and distributional moments equal to their initial values. This adds a term \( I(c_{\text{ref}} - c) \) to the source term \( f(t, z, \ldots) \) in (4.13), with \( c \) representing \( X_N, X_p, V \) and the raw moments of the biomass distribution. The flow rate is set to a low value (0.086 d\(^{-1}\)), ensuring that it has little direct effect on the concentrations of mass variables; it primarily guarantees a base level of biodiversity (i.e., trait distribution variance), on which selection can then operate (Levin 1998). The final system of partial differential equations is solved numerically by the tracer framework of the physical model.
4.3 **Results**

4.3.1 **Mass variables**

A high-level overview of system developments is provided by the changes in mass variables, such as would be present in traditional ecosystem models: the concentration of nutrient, biomass and organic matter. Seasonal changes in light- and mixing intensity govern the conspicuous changes in these variables: in early spring, when the light intensity continues to increase (Figure 4.1a) and winter mixing has subsided (Figure 4.1b), a plankton bloom develops in the top 100 m of the water column, resulting in local nutrient depletion (Figure 4.2a,c). Subsequently, biomass turnover causes the concentration of organic matter to increase (Figure 4.2b). After two more months the concentration of organic matter has decreased again, indicating the presence of (partial) heterotrophs. This does not affect the concentration of structural biomass, which remains high over summer. Only at the increase in mixing intensity in autumn (due to the onset of storms that cool and shear the surface, producing turbulence) and the gradual decrease in light intensity, the bloom is finally terminated: as surface water is mixed with deep, nutrient-rich waters, concentrations of biomass and organic matter drop whereas the nutrient concentration rises. Simultaneously the light intensity as experienced by the plankton drops sharply, because of the seasonal decrease in solar radiation, but more importantly because the high mixing intensity cause the plankton to spend more time in deeper, darker water. This dark environment cannot support autotrophy, preventing the biomass remineralized in maintenance from ultimately being rebuilt; as a result the structural biomass of the plankton community drops to background levels.
4. An adapting ecosystem manoeuvring between autotrophy and heterotrophy

Figure 4.2. Concentrations of nutrient (a), dead organic matter (b), and structural biomass (c) as a function of time (horizontal) and depth (vertical), over a one year period. Only the top 250 m of the water column is shown; from this level onward concentrations do not change.
Changes in the distribution of autotrophy and heterotrophy as a function of time (horizontal) and depth (vertical), over a one year period. Shown respectively: the mean relative investment in autotrophy (a), the mean relative investment in heterotrophy (b), the standard deviation of the relative investment in autotrophy (c), the standard deviation of the relative investment in heterotrophy (d), and the correlation between relative investments (e). Colour scales are normalized to the reference values (i.e., initial and immigration values), so that white signifies the reference value, red signifies an elevated value compared to the reference, and blue signifies a reduced value compared to the reference.
4.3.2 Community structure

Non-correlated changes in nutrient, biomass and organic matter concentrations already suggest that the structure of the plankton community changes in time and space. However, a much more detailed picture emerges from the development of the moments of the trait distribution, i.e., the mean, standard deviation and correlation of the distribution of investments in autotrophy and heterotrophy (Figure 4.3). The means characterize the strategy of the community as a whole, in terms of the investment in autotrophy and heterotrophy averaged over the complete ensemble of species. Standard deviations represent measures of biodiversity, in terms of variation in the relative investment in autotrophy and heterotrophy. The correlation between autotrophy and heterotrophy contains valuable information on individual species: a positive correlation implies both strategies are preferably combined in a single mixotrophic species, whereas a negative correlation suggests the presence of separate specialized autotrophs and heterotrophs. In all distributional moments one can recognize distinct patterns in space and time. In many of these patterns changes in time appear independent of changes in space: the trends persist when selectively integrating over time or space (Figure 4.4), allowing us to study the effects of temporal and spatial segregation in isolation.

4.3.3 Temporal changes in community structure: seasonal succession

Seasonal changes in community structure are most pronounced in the surface layer, which exhibits the greatest temporal variability in resource availability (Figs 4.1a, 4.2a, 4.2b). During the course of the year, the dark, nutrient-replete winter situation is replaced in spring by a stratified, well-lit, depleted regime, undone only in autumn as turbulent mixing strongly diminishes the effective light availability and provides access to the deep nutrient pool. These changes in light availability are directly reflected in the mean investment in autotrophy (Figs 4.3a, 4.4a), which gradually increases during the dark months, but starts to decline directly after the column becomes stratified and better lit. This decline lasts till autumn, when the near-surface autotrophic investment has dropped to a third of its early spring value. On the other hand, the mean investment in heterotrophy reaches a minimum in the first quarter (Figs 4.3b, 4.4b), after months of continued decrease in ambient organic matter (Figure 4.2b). Only after the plankton community is well-established and produces non-negligible amounts of organic matter, the mean heterotrophic investment recovers rapidly to three times its minimum value in later spring/early summer. When viewed in combination, the changes in mean autotrophic and heterotrophic investment succinctly describe the classic shift from an assemblage of primarily autotrophic species (e.g., diatoms) in early spring (Blight et al. 1995; Chang et al. 2003; Margalef 1958) to a community composed of mixotrophic and heterotrophic species (e.g., dinoflagellates) over the course of summer (Chang et al. 2003).
4.3 Results

Additional information on seasonal changes in community composition is present in the patterns in the standard deviation and correlation between traits. The standard deviation of the investment in autotrophy shows a maximum in early spring, supporting the observation that algal diversity peaks just before the onset of the spring bloom (Aubry and Acri 2004; Trifonova 1993) and decreases afterwards (Chang et al. 2003). The standard deviation of the investment in heterotrophy shows a minimum in that same period and a considerable subsequent increase. As such it mimics the real-world assembly of a diverse community of mixotrophs and heterotrophs over the course of summer (Chang et al. 2003). More intriguingly, the correlation between the autotrophic and heterotrophic investments shifts from slightly but distinctly positive (0.09) in the first months of the bloom, to negative (-0.09) at the end. This tentatively indicates that the initial increase in mean heterotrophic investment is due to the appearance of mixotrophic species, whereas in later months specialized species such as pure heterotrophs (e.g., bacteria) appear.

4.3.4 Depth-dependent community structure

The community structure varies considerably with depth (Figs 4.3, 4.4), which is readily explained by the depth-dependent light availability (Eq (4.12)). Most prominent is a fourfold increase in mean autotrophic investment between the surface and 120 m depth (Fig 4.3a, 4.4c), suggesting the presence of a shade flora (Sournia 1982b) that has a cellular chlorophyll content four times higher than that of the surface community. This is a plausible range of cellular chlorophyll (Cloern et al. 1995). The product of the mean autotrophic investment (increasing with depth) and structural biomass (decreasing with depth) represents autotrophic biomass, a measure of the chlorophyll concentration. This compound variable has a maximum at 80 m depth (not shown) with threefold the surface value; both this depth and range are characteristic for the simulated site (Steinberg et al. 2001).

With the increase in the mean autotrophic investment with depth, the standard deviation of this trait increases as well (Fig 4.4c). This suggests that the diversity of the deep algal community is higher than that of the surface community. The greatest change in algal diversity occurs between 50 and 100 m: the depth of the chlorophyll maximum. This agrees perfectly with the observation that this maximum separates a low-chlorophyll surface community that is low in diversity from a more diverse high-chlorophyll “shade flora” (Venrick 1982). Turning to heterotrophy, we may observe that though the variation of the trait mean with depth characterizes the community strategy, it cannot disentangle co-occurrence of autotrophic, mixotrophic and heterotrophic species. Only in combination with the depth-dependent correlation of traits this is feasible: with increasing depth, the correlation between autotrophic and heterotrophic investment decreases to become distinctly negative (-0.17) at 100 m depth (Fig 4.3e). This suggests a trend of increased specialization with depth, corroborating the observation that mixotrophy is restricted to surface waters (Sanders et al. 2000; Sonntag et al. 2006) and is nearly absent in the chlorophyll maximum (Arenovski et al. 1995).
4. An adapting ecosystem manoeuvring between autotrophy and heterotrophy

![Figures 4.4](image)

**Figure 4.4.** Depth-averaged (a,b) and time-averaged (c,d) distribution of autotrophy and heterotrophy, visualized as the mean and 10th and 90th percentiles of the respective marginal distributions. Note that percentiles are calculated from the distributional mean and variance under the assumption that traits are log-normally distributed (as is assumed for the model derivation). Reference values used for initialization and immigration are shown in blue.

### 4.4 Discussion

#### 4.4.1 General patterns

A defining characteristic of the spatiotemporal variation of the trait means is the existence of an optimum investment in resource harvesting, dependent on resource availability. If resource availability is negligible, investment in its retrieval is never profitable and will tend to zero (e.g., the mean heterotrophic investment in spring). On
the other hand, if a resource is relatively abundant – e.g., when another resource is limiting growth –, a low harvesting investment suffices. This causes the often counterintuitive decrease in harvesting investment where the associated resource is abundant (e.g., the mean autotrophic investment in the well-lit but nutrient-depleted summer). Only when an increase in resource retrieval could significantly enhance population growth, the harvesting investment will actually increase (e.g., the mean autotrophy at 120 m depth, the mean heterotrophy in summer). One result of this behaviour is that the community will tend to those investment coefficients that optimize the balance between the internal arrival rates of complementary resources, such that the growth rate is maximized while a minimum of retrieved resources remains unused. Arguably this is a direct result of the investment trade-off incorporated in the model. However, the model assumes simple linear relationships between the investment in resource retrieval and its internal availability (Eq (4.1), (4.2)), cost for maintenance (Eq (4.4)) and cost for growth (Eq (4.3)), and as such could be considered to embody the canonical trade-off for investment-dependent resource harvesting. The tendency to tune investments in resource harvesting in order to balance internal resource arrival rates according to resource requirement could therefore be a structural feature of natural systems.

Figure 4.5. Difference between results obtained with the approximate model (AM), and results obtained with a reference simulation of the discretized full model (FM). Deviations are taken over the final simulated year, interpolated to a regularly spaced grid with $\Delta z=1 \text{ m}$, $\Delta t=1 \text{ d}$, in the euphotic zone defined as the region where $V > 0.004 \text{ \mu M}$ for the FM; this is typically the case in the top 150 m of the column. Deviations for a given variable are measured in % of its relevant range, i.e., the range of values taken by the variable in the results of the FM. Positive deviations indicate overestimation by the AM compared to the FM, negative deviations indicate underestimation.
Standard deviations of the traits also exhibit characteristic patterns. They roughly follow the mean, which implies that the relative variation is preserved. As a consequence, the assumption of a constant coefficient of variation might simplify the present system while preserving some key behaviours, whereas the assumption of a constant variance of traits (Abrams et al. 1993; Wirtz and Eckhardt 1996) would likely fail. The main exception to the pattern of constant relative variation is found in the high standard deviation during the main regime shift, i.e., when the spring community of autotrophs is replaced by a summer community of mixotrophs and heterotrophs. This is intuitively easy to understand: during major shifts in species composition, members of both communities are present and biodiversity is high.

4.4.2 Quality of approximation

The present approach describes the behaviour of a continuum of autotrophs, mixotrophs and heterotrophs, characterized by the mean and covariances of the distribution of autotrophy and heterotrophy. In the reduction from the full model (FM) with an infinite number of species to the approximate model (AM) based on distributional moments, several approximations are made: (1) third- and higher-order derivatives of the specific growth rate to the log-transformed traits are neglected, (2) the skewness and kurtosis of log-transformed traits are estimated from relations valid for the normal distribution, and (3) moments of the untransformed traits are calculated from moments of the log-transformed traits under the assumption that the trait distribution is log-normal (chapter 3). These approximations considerably simplify the model, but they also introduce errors: the behaviour of the AM will deviate from the behaviour of the FM. To estimate the scope of this deviation, we additionally solve the FM numerically by discretizing the bivariate distribution on a 50 x 50 logarithmically spaced grid. The behaviour of the resulting ensemble of 2500 species is compared to that of the AM in Figure 4.5. Foremost one can observe that higher moments suffer from larger deviations: the deviation for structural biomass is very small (> 50 % of the results has < 1.8 % deviation), larger for the mean (> 50 % of the results has < 9.6 % deviation), and at times high for the covariances (> 50 % of the results has < 25 % deviation). This tendency for errors to increase for higher moments is a direct result of the first two approximations, which affect higher moments in particular (see also chapter 3). In view of the deviations, we would argue that the approximate results for the structural biomass and the trait means can serve quantitative purposes, whereas results for the covariances primarily should be judged qualitatively – the qualitative behaviour of covariances in the FM and AM is identical. On the whole, we conclude that the applied approximations perform well, as the resulting 8-dimensional approximate model ($V_T, X_N, X_D, \mu_L, \mu_D, \sigma_{LL}, \sigma_{DD}, \sigma_{LD}$) summarizes the behavior of the full model represented by 2500 species and 2 resources with good accuracy; this allows for a reduction from 250200 to 800 state variables in the 100-layer vertically-explicit setup.
4.4.3 Complex Adaptive Systems

The present work can be interpreted as a typical example of Complex Adaptive Systems (CAS) theory (Holland 1996; Levin 1998), which aspire to understand the dynamics of aggregate community variables from the simple rules that govern the behaviour of individual community components. CAS can be characterized by three features: (1) sustained diversity and individuality of system components, (2) localized interactions between components, and (3) an autonomous process that selects components based on the outcome of the interactions (Levin 1998). In the present model each of these features is present: the diversity of a continuum of individual species is guaranteed by a continuous inflow of trace amounts of all possible species, interactions between species – in the form of competition for shared nutrient- and organic matter pools – are localized in vertical space and time, and natural selection determines the outcome of interspecific competition.

Immigration is an essential component in the present model. In the absence of immigration, competitive exclusion causes most diversity to be lost within the first simulated year (i.e., variances tend to zero, not shown). This characteristic loss of diversity (Bruggeman and Kooijman 2007; Loreau and Mouquet 1999; Norberg et al. 2001) occurs notwithstanding the temporally variable forcing and the spatial structure, both factors that can promote coexistence (Chesson 2000). The immigration component is thus essential for realistic model behaviour. However, natural aquatic systems are indeed thought to be shaped for an important part by immigration (Cloern and Dufford 2005; Leibold and Norberg 2004), and the same has been argued for other environments (Polis et al. 1997). Thus, the inclusion of immigration is not just an artificial means of maintaining diversity. Also the diverse background community that immigration effectively creates is in fact a well-known feature of communities of small species (Fenchel and Finlay 2004). Therefore we would argue that the incorporation of a background diversity in modelling frameworks, e.g., the System of Infinite Diversity (Bruggeman and Kooijman 2007) is at least for small species justifiable.

In the present setup, species interact indirectly by competing for shared resources, i.e., inorganic nutrients and organic matter. These interactions are localized in vertical space: interactions are specific to each depth, and their result is only partially transmitted to other depths through diffusion. Spatial segregation proves an important factor in the characteristic behaviour of the system in time: in a depth-integrated model the observed ranges of the trait means and covariances are notably smaller (and all spatial patterns obviously remain unresolved), similar to earlier work (Bruggeman and Kooijman 2007). One may also realistically argue that interactions between species are localized in time: the imposed temporal variation in light- and mixing intensity causes the fitness landscape to change, even independent of species-induced modification (e.g., resource depletion) of the environment. In the presence of a base level of diversity, this temporal variability of the environment guarantees
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continual adaptation, perpetual novelty and far-from-equilibrium dynamics – all identified as emergent properties of CAS (Levin 1998).

4.4.4 Adaptation, succession and evolution

The trait value distribution in natural systems can evolve for a variety of reasons: (1) physiological adaptation changes the trait value of individuals during their life span, (2) succession changes the trait value distribution of a community or ecosystem on ecological time scales (one to a few generations), and (3) genetic evolution changes the trait distribution on evolutionary times scales (many generations). In several respects these mechanisms are very similar. Succession and evolution in particular result both from selective forces operating on an ensemble of populations that differ in trait value; they differ primarily in the origin of diversity: in evolution, the intrinsic, stochastic process of mutation generates genotypic diversity, which translates into the phenotypic diversity on which natural selection operates. In succession, diversity has to be maintained within the system (e.g., through spatiotemporal variation), and can otherwise increase only due to extrinsic processes, e.g., immigration from neighbouring systems.

Given a level of diversity, the dynamics of the mean \( \bar{x} \) of some trait \( x \) are identical for succession as well as evolution:

\[
\frac{d\bar{x}}{dt} = \nu \frac{\partial r}{\partial x},
\]

in which \( r \) represents a fitness measure (commonly the specific growth rate) and \( \nu \) a measure of "biovariability": the variance of the stochastic process of mutation for evolution (Dieckmann and Law 1996) or the deterministic variance within the community for succession (Norberg et al. 2001; Wirtz and Eckhardt 1996). In addition, it has been argued that physiological and behavioural adaptation may be subject to the same dynamics; the biovariability \( \nu \) then comes to represent a generic capability to adapt (Abrams et al. 1993). Despite the similarity in dynamics, changes on ecological and evolutionary time scales have traditionally been regarded as different disciplines; only recently petitions for integration of these fields emerged (Fussmann et al. 2007). We feel that the present study demonstrates several principles that could contribute to this process of integration: (1) the mechanisms that underlie trait value change are explicitly formulated on the level of organization at which diversity in generated (for succession this is the population, for physiological adaptation and evolution the individual organism), before an approximation for dynamics of trait distribution characteristics is derived, (2) trait covariances are resolved explicitly to account for the history of the system as well as mechanisms affecting diversity (e.g., immigration or mutation), and (3) the accuracy of the approximation for trait distribution dynamics is evaluated through simulations of the full model (e.g., by discretizing the trait distribution or stochastic simulations). The strength of a formulation in terms of first principles and combined with resolution of covariance dynamics has previously been convincingly demonstrated by Nuismer et al. (2005).
4.4.5 Final thoughts

The present results demonstrate that patterns in traditional ecosystem variables – nutrient, organic matter, biomass – provide little beyond a crude indication of the changes that occur within the plankton community. It is the incorporation of the trait distribution that enables the resolution and explanation of a wealth of aquatic phenomena. The additional reduction of the trait distribution to its mean and covariances allows for a considerable reduction in computational cost, while preserving key features of the distribution with reasonable accuracy. The final minimal model (7 physiological parameters, 8 state variables per point in space) reproduces known patterns in mass variables, community strategy and biodiversity. Such combined predictions are traditionally the domain of complex, underdetermined food web models. Trait-based approaches offer an alternative to such models, combining a minimum of physiological detail with predictive capabilities for a wide range of ecosystem aspects.

4.5 References


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5 A generic method for estimation of trait values using phylogeny


Abstract
A wealth of information on metabolic parameters of a species can be inferred from observations on species that are phylogenetically related. Phylogeny-based information can complement direct empirical evidence, and is particularly valuable if experiments on the species of interest are not feasible. The PhyloPars web server provides a statistically consistent method that combines an incomplete set of empirical observations with the species phylogeny to produce a complete set of parameter estimates for all species. It builds upon a state-of-the-art evolutionary model, extended with the ability to handle missing data. The resulting approach makes optimal use of all available information to produce estimates that can be an order of magnitude more accurate than ad-hoc alternatives. Uploading a phylogeny and incomplete feature matrix suffices to obtain estimates of all missing values, along with a measure of certainty. Real-time cross-validation provides further insight in the accuracy and bias expected for estimated values. The server allows for easy, efficient estimation of metabolic parameters, which can benefit a wide range of fields including systems biology and ecology. PhyloPars is available at: http://www.ibi.vu.nl/programs/phylopars/.
5.1 Introduction

Quantitative predictions on the behaviour of organisms, populations and ecosystems require accurate values for the metabolic parameters associated with cellular and physiological processes. These parameters range from the substrate affinities, processing rates and yield coefficients of single enzyme-mediated chemical reactions, to the growth rate and maintenance requirement of individual organisms or populations. Ideally, such parameters are measured directly by observing the species (or strain) of interest in experiments. However, this can be a costly, time-consuming and difficult process. It may even be impossible: many species that play key roles in nature have never been successfully kept in culture or captivity. In such contexts, methods that exploit alternative information sources to estimate parameter values can be very valuable. One such source of information is found in direct observations on phylogenetically related species: given that evolution changes most features gradually over time, two species that separated recently in evolutionary history would be expected to behave similarly. The best estimate for a metabolic parameter could thus be derived from observations on related species.

Intuitively, one might expect that the best estimate for a missing parameter is given by the observed value of the most closely related species available. Certainly, evolutionary models generally agree that the best estimate for the parameter of a species is given by the closest node possible: the true parameter value of its parent in the phylogeny (Felsenstein 1973). However, this value is usually unknown. First, the parent may be extinct, in which case we can only obtain indirect information on its original parameter value by sampling descendants. Second, most observations are samples subject to measurement error, rather than perfect measurements of the true value. Therefore, any empirically available estimate of the parent value is subject to error. We can reduce this error by considering more distantly related species in the phylogeny: every sampled species in the phylogeny tells a little about the possible value of the missing parameter. An optimal reconstruction of the parameter value thus combines observations throughout the phylogeny, weighed according to phylogenetic proximity. This is a dominant idea in comparative feature analysis (Felsenstein 1985; Lynch 1991) and ancestral state reconstruction (Cunningham et al. 1998; Garland et al. 1999; Schluter et al. 1997), and occasionally surfaces in other applications such as sequence alignment (Altschul et al. 1989; Vingron and Sibbald 1993) and comparative sequence analysis (Stone and Sidow 2007).

Another source of information on the value of a missing parameter may be found in other observations on the species of interest: its other features may tell a lot about the missing value. A prime example is the maximum body size of species, which is commonly associated with a plethora of features through theory for metabolic organization (Kooijman 2000) and empirical allometric scaling laws (West et al. 1997). A good indication of the value of certain metabolic parameters could therefore be given by the size of the species, or in fact any observed parameter that is known to correlate with the feature of interest. It is tempting to identify and use such
correlations directly through regression analysis applied to observations across species. However, such observations are not independent due to interspecific phylogenetic relationships, leading to overestimation of the correlations (Felsenstein 1985). Information on parameter correlations can provide a valuable aid for reconstructing missing parameter values, but strikingly, their identification and use again requires a phylogeny-aware analysis.

Figure 5.1. An example of a phylogenetic tree with five species (A-E), two features (red and blue numbers) and one missing value (question mark). PhyloPars reconstructs the missing value from the other observed values of that feature (red numbers) weighed according to phylogenetic proximity, and additionally involves the observed value of the other feature (blue value 5) through its estimate of the phylogenetic correlation between the two features. This estimate is in turn based on all observations. Simple ad-hoc approaches typically do not make such complete use of available information: they use the average of the other observed feature values (red numbers only) as estimate (“mean model”), or insert the phylogenetically nearest observed value: the value 1 observed for species D (“nearest neighbour model”).

The PhyloPars web server offers an efficient, statistically consistent method that exploits both phylogenetic relationships and parameter correlations to estimate missing parameters of the species within a phylogeny (Figure 5.1). It builds upon a state-of-the-art model (Felsenstein 2008; Ives et al. 2007) that additionally accounts for intraspecific variability and measurement error. This model is extended to handle missing data. The resulting approach makes optimal use of all available observations to produce estimates that can be an order of magnitude more accurate than ad-hoc alternatives.

5.2 Underlying model

PhyloPars operates on a phylogeny and an incomplete feature matrix that describes the available observations on one or more continuous features (e.g., metabolic parameters), for subsets of nodes (species or strains) that may fully or partially overlap. The phylogeny is assumed to be known in terms of both topology and branch lengths; the latter are assumed to be proportional to evolutionary time.
5.2.1 Phylogenetic variability

The role of the phylogeny is represented by a “Brownian motion” phylogenetic model that assumes feature values change through genetic drift (Felsenstein 1973; Felsenstein 2008; Lynch 1991; Revell and Harmon 2008; Stone and Sidow 2007). A consequence of the model is that all feature values for all nodes combined can be described by a single multivariate normal distribution. The covariances of the distribution depend on the topology and branch lengths of the phylogeny, and on the rates and correlations of the evolution of the different features. These rates and correlations are described by $N(N+1)/2$ “phylogenetic” covariances (Felsenstein 2008), with $N$ denoting the number of features. They are easily transformed into more readily interpretable phylogenetic regression slopes (Garland and Ives 2000; Lavin et al. 2008) and phylogenetic correlations (Felsenstein 2008). It is worth noting that the term “phylogenetic correlation” has been used to describe different concepts (Blomberg et al. 2003; Felsenstein 2008); we follow Felsenstein in using it exclusively to refer to joint evolution of a pair of features.

5.2.2 Phenotypic variability

The phylogenetic model is extended to account for phenotypic variability: the fact that a single sample is not necessarily the mean of the species under study (Felsenstein 2008; Ives et al. 2007). Such variability may be due to measurement error or to intraspecific variation of the feature. It can be incorporated in the phylogenetic model by introducing a layer of variability between the species level and the observation, effectively behaving as extension of the evolutionary path (Felsenstein 2008). This is comparable to the role of non-heritable residual variability in phylogenetic mixed models (Housworth et al. 2004; Lynch 1991).

We assume that observed correlations between features are exclusively due to evolutionary processes (and not, for instance, to the measurement process itself). This facilitates extending the model with the ability to use incomplete observations, i.e., observations on a species that include only a subset of all features. As observations may originate from different sources, with sets of observed species per feature not necessarily overlapping, this functionality is indispensable for many purposes. Phenotypic variability is assumed equal for all species (but can differ between features), and is described by $N$ unknown “phenotypic” variances (Felsenstein 2008).

It may be noted that this differs from the approach taken by Ives et al. (Ives et al. 2007), who permit phenotypic variability to differ between species (as well as between features); values for the phenotypic variability are there prescribed rather than estimated.

5.2.3 Procedure

Both the phylogenetic covariances and the phenotypic variances are initially unknown and need to be estimated from the input data in order to reconstruct missing feature values. This is typically done through maximum likelihood estimation (MLE) (Felsenstein 2008; Ives et al. 2007; Lynch 1991; Revell and Harmon 2008).
With the phylogenetic and phenotypic covariances known, estimation of missing parameters is straightforward: the optimal phylogenetic and phenotypic covariances are first combined with the tree topology to calculate the covariances between the observations and the missing values. These are subsequently used to express the estimate of each missing value as the product of all original observations and an estimate-specific set of associated weights (formally: regression coefficients).

In order to assess the validity of the model result, one can additionally perform cross-validation: each observed parameter is excluded from the input data, and then re-estimated with the MLE-derived phylogenetic and phenotypic covariances to determine prediction error and bias.

5.3 Web server implementation

5.3.1 Input
The web server accepts an uploaded phylogeny in Newick format (http://evolution.genetics.washington.edu/phylip/newicktree.html) and a feature matrix with observations as tab-separated text file. The latter can contain missing values. If there is good evidence that either phylogenetic correlations or phenotypic variability are absent in the input dataset, the user can additionally disable correlated evolution of features (phylogenetic correlations will be set to zero) or phenotypic variability (phenotypic variances will be set to zero), respectively. This restricts the freedom of the model and will then correctly decrease the uncertainty associated with estimated missing values.

5.3.2 Processing
The web server first constructs the full multivariate normal model that specifies the likelihood of observing the provided feature matrix, given the phylogeny, phylogenetic covariances and phenotypic variances. The covariance matrix of the model combines phylogenetic and phenotypic components in such a way that analytic calculation of the optimal phylogenetic and phenotypic covariances is not possible (Felsenstein 2008; Ives et al. 2007). Therefore, we resort to iterative numerical maximization of the likelihood. Phylogenetic and phenotypic covariances are first transformed into a set of unbounded parameters through log Cholesky parameterization (Pinheiro and Bates 1996); this permits unconstrained optimization. The likelihood is then maximized with the Broyden-Fletcher-Goldfarb-Shanno algorithm (Nocedal and Wright 2006).

All processing logic is implemented in Python (http://www.python.org). For optimization and advanced linear algebra we use SciPy (http://www.scipy.org), which in turn encapsulates LAPACK (Anderson et al. 1999). All output plots are generated with MatPlotLib (http://matplotlib.sourceforge.net). A mathematical description of the methodology is provided as online supplementary information. Total processing time depends on the number of features and nodes under study; a test case with 242 nodes, 6 features and 289 observations is processed in under 3 minutes.
5.4 Worked example

We have applied the PhyloPars method to an extensive database of freshwater phytoplankton parameters. Phytoplankton represent the lowest trophic level in aquatic food webs, and as such govern processes on all scales: from small lakes to the global climate. Their influence is hard to quantify as many plankton species cannot be cultured. This therefore presents an ideal test case for the PhyloPars approach.

The dataset was compiled by J.B. from 38 literature sources and contains over one thousand measurements on 12 different features of 114 species. For the present study we have selected a subset of features: cell length, diameter, surface area, volume, maximum growth rate and phosphate affinity. It may be obvious that the first four features all describe aspects of cell size, and are likely to be positively correlated. Their joint inclusion is intentional: it demonstrates the ability of PhyloPars to uncover and exploit correlations between features.

To our knowledge, there does not exist a complete phytoplankton phylogeny based on molecular evidence. Therefore, we resort to using the Linnaean taxonomy with branch lengths of 1 between ranks. While this is undoubtedly a very crude approximation to the topology and branch lengths of the true phylogeny, other work indicates that even such qualitative phylogenies can contribute information on feature evolution (Martins and Garland 1991).

The sample feature matrix contains a total of 289 observed values for a total of 242 phylogenetic groups (species and ancestors), leaving 1163 missing values. Both the feature matrix and phylogeny are available at the PhyloPars home page. Results obtained with default settings are shown in Figure 5.2.
5.4 Worked example

Figure 5.2. Output of the PhyloPars web server consists of three sections: (A) estimates for phylogenetic and phenotypic variability, (B) estimates for missing parameter values, and (D) cross-validation details. Individual parameter estimates can be clicked to obtain a detailed report in a pop-up window; an example for the maximum growth rate of Chroococcus is shown in (C).
5.4.1 Phylogenetic and phenotypic variability

In the first section of its results (Figure 5.2A), PhyloPars presents maximum likelihood estimates for the phylogenetic and phenotypic variability. Phylogenetic standard deviations provide a measure of the rate of feature evolution. Phenotypic standard deviations quantify the variability due to measurement error and/or intraspecific variation. The proportion of variance accounted for by the phylogeny is also presented, and may be used to compare phylogenetic and phenotypic contributions to the total observed variability (Housworth et al. 2004). This proportion usually includes a contribution by natural selection (Westoby et al. 1995); further analyses (Cubo et al. 2005; Desdevises et al. 2003) might be used to disentangle phylogenetic and selection components. For reference, the table also lists a summary of cross-validation results (see below). Finally, phylogenetic correlations are shown; these indicate if pairs of features are likely to co-evolve.

For the phytoplankton example phylogenetic variability clearly plays an important role: the phylogeny explains more than 50% of the total variability of all features. It is also apparent that PhyloPars correctly recognizes likely correlations between features: correlations between length, diameter, surface area and volume all exceed 0.5.

5.4.2 Estimates for missing values

In the second result section (Figure 5.2B), estimates for all features of all nodes are presented in one single “supplemented” feature matrix. Feature values that are also present in the input data as observation are indicated by a trailing asterisk. It is worth noting that the estimated value of a parameter may differ from its original observation when phenotypic variability is allowed: in that case the observation is a single sample, whereas the supplemented feature matrix lists the expected (mean) value for the representative species. The supplemented feature matrix is also available as a downloadable tab-separated text file.

Clicking on a value in the supplemented feature matrix opens a detailed report (Figure 5.2C) that visualizes the contributions of all observations to the point estimate (black vertical bars and blue area). Additionally, it presents the standard deviation of the estimate. Together the point estimate and standard deviation specify the marginal likelihood of the estimated value (a normal distribution), plotted as a red curve.

Results for the example clearly demonstrate that estimates generally differ even for closely related species (e.g., *Anabaena* spec.) – this is a direct result of the PhyloPars capability to include observations on other features in its estimates through phylogenetic correlations.

5.4.3 Cross-validation

In the last result section (Figure 5.2D), detailed cross validation reports are presented. These visualize the distribution of estimation errors, i.e., the differences between
observations and their estimates in cross-validation. Error distributions are also plotted for two simple ad-hoc models: a mean model that assumes the best estimate for a missing value is given by the mean of all observations (valid if phylogenetic variability is absent), and a nearest neighbour model that assumes the best estimate for a missing value is given by the phylogenetically closest observation (a common method of estimating unknown parameters). These allow the user to judge the improvement of the PhyloPars model over the ad-hoc models. Values are also presented for the expected bias (the mean of all differences between estimates and observations in cross-validation), and the expected error (the mean of all absolute differences). These provide an indication of the accuracy of the estimates for missing values.

For the example, neither of the ad-hoc models has a definite advantage over the other, and the PhyloPars evolutionary model always improves upon both. This improvement can be very large: the mean error in the estimate for cell surface area is 25% compared to over 300% for the ad-hoc models. Additionally, the bias of the PhyloPars model is near zero for all features: a definite improvement over the nearest neighbour model (the mean model has no bias by definition, but its errors are relatively large).

5.4.4 Discussion and conclusion

PhyloPars delivers estimates of missing feature values that can be an order of magnitude more accurate than those of ad-hoc alternatives. The maximum precision achievable depends in part on the accuracy of the topology and branch lengths of the user-supplied phylogeny. For a limited number of species, accurate phylogenies based on molecular evidence are available. For instance, TreeFam (Ruan et al. 2008) and Pfam (Finn et al. 2008) offer phylogenetic trees based on gene and protein similarity, respectively. Branch lengths can then to some extent be expected to represent evolutionary time. If a detailed phylogeny is not available for the species of interest, a qualitative tree derived from resources such as the NCBI taxonomy (Sayers et al. 2009) could be used instead. The worked example demonstrates convincingly that even a taxonomy-based phylogeny with arbitrary branch lengths allows PhyloPars to improve considerably upon alternative models.

A valid concern is to what extent the accuracy of PhyloPars predictions depends on the underlying “Brownian motion” evolutionary model. It has been argued that this model overemphasizes the randomness of evolutionary change, at the expense of directional change due to natural selection (Westoby et al. 1995). Not surprisingly, several alternative models of evolution have been proposed (Blomberg et al. 2003; Mooers et al. 1999). However, the mathematical framework that underpins the Brownian motion model can be motivated independently on first-principle statistical grounds (Garland and Ives 2000; Grafen 1989). Accordingly, the model has been shown to deliver accurate predictions even for data generated with alternative evolutionary models (Martins et al. 2002). If no detailed information is available on
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the processes that governed evolutionary change, the Brownian motion model provides a robust base model for phylogenetic analyses.

Within the context of the Brownian motion evolutionary model, the best estimate for a feature is given by that of its parent in the phylogeny. Estimating missing feature values thus equates to reconstructing ancestral states. Several stand-alone applications are capable of this, e.g., Pagel’s BayesTraits (http://www.evolution.reading.ac.uk), Swofford’s PAUP (http://paup.csit.fsu.edu), and Mesquite with the PDAP-PDTREE package (http://mesquiteproject.org). However, none of these applications incorporates phenotypic variability of features, which plays an important role in practice (Felsenstein 2008; Ives et al. 2007), and several do not accept datasets with missing values or cannot process these reliably. The “contrast” program in Felsenstein’s PHYLIP (http://evolution.genetics.washington.edu/phylip.html) deserves special mention, as it performs all pre-processing needed for subsequent ancestral state reconstruction and can handle phenotypic variability. However, it again does not permit missing values, which for our example would imply that only 18 out of 289 observations (3 species out of 114) could be used.

To our knowledge there does not exist a stand-alone or web application that offers a straightforward means of performing the complex task of phylogeny-based reconstruction of missing parameter values, comparable in ease of use and visual support to that offered by the PhyloPars web server. PhyloPars for the first time discloses valuable, theoretically advanced methods from evolutionary biology to experimentalists and modellers alike. Its results can serve several purposes: (1) estimates may be used directly to predict the behaviour of species, populations or ecosystems, (2) quantitative models can use PhyloPars predictions to supplement existing knowledge, either by directly incorporating a subset of its estimates or by using the predicted marginal likelihood as prior distribution in Bayesian context, (3) estimates can aid experimental design by providing a prior indication of the feasible range for metabolic parameters. We feel that such functionality may benefit a wide range of fields, including ecology and systems biology.

5.5 Appendix: methodology

5.5.1 Introduction

PhyloPars reconstructs missing feature values of the nodes (species or strains) of a phylogeny, using a limited number of observations. The main idea behind the method is that the closer related a node is, the more it will tell us about a missing feature value. Specifically, feature values are assumed to change through genetic drift only, with the rate of change (mutation) being constant for the entire phylogeny. Evolutionary changes in the value of different features are allowed to be correlated, such as would be the case for the change in length and surface area, for instance. Additionally, the model allows for phenotypic variability of features: the fact that an
observation or measurement is not necessarily the exact feature value of the representative node. This may be the case when there exists within-species or within-strain variation of the feature value, or when observed values are affected by measurement error.

The phylogenetic model used is the wide-spread "Brownian motion" model of evolution (Felsenstein 1973; Felsenstein 1988), formulated for multiple features (1985; 2008; Lynch 1991). Phenotypic variability is added as an additional layer of variability between the species and sample level. The level of phenotypic variability is taken be feature-specific and constant across the phylogeny; its value is estimated from the observations (Felsenstein 2008). This contrasts with the approach by Ives et al (Ives et al. 2007), who allow for a variable (node-specific), pre-specified phenotypic variability. Conceptually the PhyloPars methodology is nearest to that employed by Felsenstein (Felsenstein 2008), but it differs in two aspects. First, PhyloPars assumes different observations on a single species to be independent, which formally implies that phenotypic correlations equal zero. Second, the model is extended with the facility of handling missing data: values in the feature matrix may be sampled 0, 1 or more times. This contrasts with the approach by Felsenstein, which requires for any sampled individual or population that all feature values are measured.

Broadly, there exist three approaches to mathematically develop and analyze the conceptual model introduced in the previous paragraph: Phylogenetically Independent Contrasts (PIC) (Felsenstein 1985; Felsenstein 2008), Generalized Least Squares (GLS) (Grafen 1989; Martins and Hansen 1997; Pagel 1997), and the Phylogenetic Mixed Model (PMM) (Housworth et al. 2004; Lynch 1991). All build upon the same assumptions and tackle very similar conceptual problems. It is therefore not surprising that they can be shown to be closely related, and to deliver identical results for some models (Felsenstein 2008; Garland and Ives 2000; Housworth et al. 2004; Rolff 2001). Perhaps the main difference between the methods lies in the questions that they typically address: both PIC and GLS are often used directly to obtain either estimates of ancestral feature values (Garland et al. 1999; Schluter et al. 1997) or to perform univariate phylogenetic regressions (Garland and Ives 2000). Accordingly, mathematical theory and analytical formulae have been developed especially for these purposes. The PMM on the other hand aims to first (numerically) reconstruct the parameters of the full evolutionary model (specifically, the phylogenetic covariance matrix), which can then serve a variety of purposes including ancestral state reconstruction, univariate and multivariate phylogenetic regression analysis, and phylogenetic principal component analysis. This led Housworth et al. (Housworth et al. 2004) to suggest that the PMM can be more informative than PIC and GLS-based counterparts. However, it should be stressed that the difference between the methods lies primarily in the typical application of the methods, and not in their base assumptions and model formulation. For instance, Felsenstein (Felsenstein 2008) uses a PIC-based method to obtain all phylogenetic and phenotypic parameters of the evolutionary model.
In a sense, PhyloPars incorporates elements from both GLS- as well as PIC-based methods. First, the complete normal multivariate model is formulated for multiple nodes and multiple traits, describing the likelihood of observing all sampled variables. This would be the starting point for a GLS analysis. Second, contrasts (but not independent contrasts) are introduced to eliminate the phylogenetic mean of the features from the problem, not unlike the approach followed by Grafen (Grafen 1989). At this point, however, the inclusion of phenotypic variability has made analytical reconstruction of the model parameters impossible – commonly used analytical expressions for the value and confidence intervals of ancestral states and phylogenetic regression coefficients do not apply. As in comparable studies (Felsenstein 2008; Housworth et al. 2004; Ives et al. 2007), numerical routines must be used to identify the parameters that maximize the likelihood.

5.5.2 Input

Let us start with a completely known phylogeny that contains a total of $M$ nodes, and a limited set of observations on $N$ features of a subset of nodes. Multiple observations on a single node are assumed to be independent (cf. Felsenstein 2008). The whole set of observations is assumed to be incomplete and may contain duplicates: any element of the $M \times N$ feature matrix may be sampled 0, 1 or more times. As the number of observations can differ between features, we define for each feature $i$ its distinct set of observations as vector $y_i = (y_{i1},...y_{ik})^T$. The indices of the node to which each observation pertains will be denoted by corresponding vector $m_i = (m_{i1},...m_{ik})^T$. The ordering of observations is irrelevant: values in $m_i$ do not need to increase monotonously. Also, as multiple observations on the value of a specific feature for a single node may be available, each $m_i$ may contain duplicates.

5.5.3 Phylogenetic variability: genetic drift

If the value of features changes through genetic drift only, features can be considered to perform a random walk in evolutionary time. This corresponds to the Brownian motion model for evolution of continuous features (Felsenstein 1973). This is by no means the only model of feature evolution (Blomberg et al. 2003; Mooers et al. 1999), but it is perhaps the simplest model possible, and it mathematical consequences can be motivated independently on first-principle statistical grounds (Garland and Ives 2000; Grafen 1989; Pagel 1993). The Brownian motion model specifies that if feature values $(x_1,...x_N)^T$ are known, the probability distribution of the feature values at time interval $t$ later is described by a multivariate normal distribution with mean $(x_1,...x_N)^T$ and covariances $a_{ij}$, with $a_{ij}$ defined as the covariance of evolutionary change between features $i$ and $j$ per unit time (i.e., branch length). Following Felsenstein (2008), we will refer to these as phylogenetic covariances. These covariances are easily transformed into phylogenetic correlations and phylogenetic regression slopes. Since the intercept of phylogenetic regressions is identical to the feature value of the root node (Garland and Ives 2000), which is reconstructed along with the values of all other nodes at the final step in the analysis, the present method also may be used to perform phylogenetic regression analyses.
Let us now consider the (rooted) phylogeny with the true value (cf., the observed value) of feature \( i \) for node \( k \) denoted by \( x_{ik} \); \( k = 0 \) will be used to denote the root of the phylogeny. The feature values of any given node have been determined by the random walk that started from the root node. Let us denote the set of branch segments that describes the evolutionary path from the root to a node \( k \) as \( P_k \), and the sum of the lengths of the segments in such a set as \( l(P_k) \). For this node \( k \) the feature values can now be described by a multivariate normal distribution with the mean equal to the feature values of the root node \( (x_{i0}, \ldots, x_{i0})^T \) and covariances equal to \( a_{ij}(P_k) \). It is not hard to see that the feature values of the different nodes must be correlated if the nodes’ evolutionary paths from the root node (partially) overlap; these nodes have shared all changes in feature values from the root till their last common ancestor. This implies that the covariance between a feature value \( x_{ik} \) and any other feature value \( x_{jl} \) is given by \( \text{Cov}(x_{ik}, x_{jl}) = a_{ij}T_{kl} \), with \( T_{kl} = l(P_k \cap P_l) \) simply equaling the length of the path from the root till the last common ancestor of both nodes.

5.5.4 Phenotypic variability: intraspecific variation and measurement error

In most cases, observations on the feature value of a given node will be subject to additional variability: different individuals of a node may have different feature values (intraspecific variability), and measurements of the feature values may be imperfect (measurement error). Following Felsenstein (2008), we will refer to these as sources as phenotypic variability. We will assume that the uncertainty due to each phenotypic source of variation can be described by a normal distribution centred at the true feature value of the respective node. As a result, the combined effect of intraspecific variability and measurement error again be described by a normal distribution, which has a mean equal to the true mean of the feature value of the node and a variance that equals the sum of the variances of the two source of phenotypic variability. We will refer to these combined variances \( b_{ij} \) as phenotypic variances. It is worth noting that as we assume that the observations on a given node are independent, phenotypic correlations are all zero (cf. Felsenstein 2008). The square root of the phenotypic variance may also be interpreted as the standard deviation expected for multiple samples taken from a single species, which thus is taken to be the same for all species (cf. Ives et al. 2007).

5.5.5 Complete model

This completes the information needed for the model specification. We now combine all observations in a single vector \( \mathbf{y} = (y_{1i}, \ldots, y_{Ni})^T \), noting that observations on a single feature thus remain contiguous. The likelihood of this set of observations equals a multivariate normal distribution that combines phylogenetic and phenotypic components.

The phylogenetic model specifies that the expected feature value of any node equals the value of the corresponding feature for the root node, while the phenotypic model
does not affect the observed mean. Thus the expectation of the distribution equals \( \bar{y} = (\bar{y}_1^T, \ldots, \bar{y}_N^T)^T \), with each \( \bar{y}_i \) denoting a vector of length \( K_i \) and elements equal to \( x_{i0} \).

Since the effect of both phylogenetic and phenotypic processes can be described by a normal distribution and the phenotypic process has a zero mean, the chaining of these processes simply results in addition of the corresponding covariances (Felsenstein 2008; Housworth et al. 2004; Ives et al. 2007; Lynch 1991). The base covariance between two observations is specified by the phylogenetic model, and incorporates a phenotypic component only if the two observations are in fact the same (i.e., only variances incorporate a phenotypic component), as phenotypic correlations equal zero. The covariance between observation \( p \in \{1, \ldots, K_i\} \) on feature \( i \) and observation \( q \in \{1, \ldots, K_j\} \) on feature \( j \) thus is given by \( \text{Cov}(y_{ip}, y_{jq}) = a_{ij}T_{m_{ip},m_{jq}} + \delta_{ij}\delta_{pq}b_{ij} \), with each \( \delta \) representing the Kronecker delta that equals 1 if its subscript indices are equal and 0 otherwise. Thus the covariance matrix may be viewed as a \( N \times N \) block matrix, with each feature-specific block \( S_{ij} \) representing a \( K_i \times K_j \) matrix containing elements \( \text{Cov}(y_{ip}, y_{jq}) \) with \( p \in \{1, \ldots, K_i\} \), \( q \in \{1, \ldots, K_j\} \). As \( a, b \) and \( T \) are all symmetric, it is not difficult to see that the resulting covariance matrix must be symmetric as well.

One could now maximize the likelihood in order to obtain the phylogenetic covariances \( a_{ij} \) and phenotypic variances \( b_{ij} \), for \( i, j = 1, \ldots, N \). However, the likelihood also contains the \( N \) unknown feature values of the root node \( x_{i0} \), which then would have to be estimated as well. This is possible and would not necessarily increase the number of free parameters, as one could “profile out” the root feature values by inserting their (analytically obtained) optimum values for any given estimate set of phylogenetic covariances and phenotypic variances. However, such joint estimation of the mean and covariance is well-known to induce a bias in the estimate of the covariances (Revell and Harmon 2008); in order to obtain an unbiased maximum likelihood estimator, we first rephrase the model in terms that do not include the root feature values.

### 5.5.6 Introducing contrasts

Following Felsenstein (1973; 1985; 2008), we first rephrase the model in terms of contrasts: the difference between two observations on the same feature. Notably, however, we use contrasts with an arbitrarily chosen reference observation, rather than independent contrasts. We set aside one observation for each feature for use as reference: from each observation vector \( y_i \) we extract one element denoted as \( y_{i0} \), reducing the vector length with 1; correspondingly we extract element \( m_{i0} \) from \( m_i \). Any element in the observation vector may be chosen as reference, which agrees with the fact the ordering of observations in \( y_i \) is irrelevant. We now define the contrast vector \( \Delta y_i = y_i - y_{i0} \) for each feature. The likelihood of observing contrasts \( \Delta y = (\Delta y_1^T, \ldots, \Delta y_N^T)^T \) again equals a multivariate normal distribution (Johnson and Kotz 1972). The mean of this distribution is a null vector, as the expectation for each \( y_{ip} \) is the root feature value \( x_{i0} \). The covariances of the contrasts can be derived from the covariances of \( y_i \) in a straightforward fashion:
\[
\text{Cov}(y_{ip} - y_{iq}, y_{jq} - y_{jo}) = E((y_{ip} - y_{io})(y_{jq} - y_{jo})) - E(y_{ip} - y_{io})E(y_{jq} - y_{jo})
\]
\[
= E(y_{ip}y_{jq}) - E(y_{ip}y_{jo}) - E(y_{io}y_{jq}) + E(y_{io}y_{jo})
\]
\[
- E(y_{ip})E(y_{jq}) + E(y_{ip})E(y_{jo}) + E(y_{io})E(y_{jq}) - E(y_{io})E(y_{jo})
\]
\[
= \text{Cov}(y_{ip}, y_{jq}) - \text{Cov}(y_{ip}, y_{jo}) - \text{Cov}(y_{io}, y_{jq}) + \text{Cov}(y_{io}, y_{jo})
\]

Inserting \(\text{Cov}(y_{ip}, y_{jq}) = a_{ij}T_{m_{ip}m_{jq}} + \delta_{ij}\delta_{pq}b_{ij}\) that was obtained previously, we get

\[
\text{Cov}(y_{ip} - y_{iq}, y_{jq} - y_{jo}) = a_{ij}(T_{m_{ip}m_{jq}} - T_{m_{ip}m_{jo}} - T_{m_{io}m_{jq}} + T_{m_{io}m_{jo}})
\]

Thus the covariance matrix for \(\Delta y\) may be viewed as a \(N \times N\) block matrix, with each feature-specific block \(S_{ij}\) representing a \(K_i \times K_j\) matrix containing elements \(\text{Cov}(y_{ip} - y_{iq}, y_{jq} - y_{jo})\) with \(p \in \{1, ..., K_i\}, q \in \{1, ..., K_j\}\). It is worth remarking that the phenotypic variances contribute first to the block diagonal (due to the use of an observed feature value as reference in the contrasts), and again to the element diagonal (due to the individual observations).

The likelihood of observing contrasts \(\Delta y\) thus equals

\[
L(\Delta y | a, b) = \frac{1}{(2\pi)^{n/2}|\Sigma(a, b)|^{1/2}} e^{-\frac{1}{2} (\Delta y - e^{\Sigma(a, b)} a)^T (\Sigma(a, b))^{-1} (\Delta y - e^{\Sigma(a, b)} a)}
\]

with \(\Sigma(a, b)\) denoting the covariance matrix and \(|\Sigma(a, b)|\) its determinant.

### 5.5.7 Estimating phylogenetic and phenotypic covariances

We now have an expression for the likelihood that depends only on the phylogenetic and phenotypic covariances. For optimization purposes it is often easier to work with the ln-likelihood, i.e.,

\[
\Lambda(\Delta y | a, b) = -\frac{1}{2} \ln 2\pi - \frac{1}{2} \ln |\Sigma(a, b)| - \frac{1}{2} (\Delta y - e^{\Sigma(a, b)} a)^T (\Sigma(a, b))^{-1} (\Delta y - e^{\Sigma(a, b)} a)
\]

The best estimates for \(a\) and \(b\) are given by those values that maximize the (ln-)likelihood. Note that the constant \(-\frac{1}{2} \ln 2\pi\) does not affect the position of the optimum of \(\Lambda(\Delta y | a, b)\) in parameter space, and can therefore be omitted.

To permit unconstrained maximization of the ln-likelihood, it is first rephrased in terms of the log Cholesky parameterization (Pinheiro and Bates 1996) of the phylogenetic covariances, and the logarithm of the phenotypic variances. This permits unconstrained optimization while ensuring that the phylogenetic covariance matrix remains positive definite, and phenotypic variances remain positive. The Broyden-Fletcher-Goldfarb-Shanno algorithm (Nocedal and Wright 2006) is then used for unconstrained minimization of the negative ln-likelihood.

The inverse and determinant of the covariance matrix \(\Sigma(a, b)\) at each evaluation of the likelihood is calculated through Cholesky decomposition of the matrix. This is the most computationally expensive step in the procedure, since the size of the (square)
matrix equals the total number of feature value observations, which may be very large (289 in the PhyloPars test case).

The likelihood maximization procedure must be provided with an initial estimate of phylogenetic covariances and phenotypic variances. To obtain such an estimate, we first calculate the optimal phylogenetic variances for each feature in the absence of phylogenetic correlations and phenotypic variability. In the absence of phylogenetic correlations, observations on different features are uncorrelated and the likelihood reduces to the product of feature-specific multivariate normal distributions. Each of these distributions has a zero mean and a covariance matrix $\Sigma_{ii}$ that depends only on the feature's phylogenetic and phenotypic variance; these components of the likelihood can therefore be maximized individually. If we neglect the phenotypic component, the feature-specific covariance matrix can be written as

$$\Sigma_{ii} = \Sigma_{A}$$

where $\Sigma_{A}$ is the covariance matrix of the trait values at the tips of the phylogenetic tree. The optimal $\tilde{\Sigma}_{ii}$ then is the one that maximizes

$$\frac{1}{2} \ln |\tilde{\Sigma}_{ii}| = \frac{1}{2} \tilde{\Sigma}_{ii}^{-1} \tilde{\Delta} y_i$$

which is found to equal

$$\tilde{\Sigma}_{ii} = \frac{\Delta y_i^T T_i^{-1} \Delta y_i}{K_i}$$

recalling that $K_i$ denotes the length of $\Delta y_i$. Further, we calculate the optimal phenotypic variances in the absence of phylogenetic variability. This is simply the variance of the observations for each feature, i.e., $\tilde{\Sigma}_{ii} = \text{var}(y_i)$, with $y_i$ taken before reference element $y_{i0}$ was extracted. As initial guess, we specify that half of the total variability is due to phylogenetic components, and half to phenotypic components. Initial estimates of phylogenetic and phenotypic variances are thus set to $\frac{1}{2} \tilde{\Sigma}_{ii}$ and $\frac{1}{2} \tilde{\Sigma}_{ii}$, respectively (recall that phylogenetic correlations are initially set to zero).

5.5.8 Reconstructing missing feature values

With phylogenetic covariances and phenotypic variances known, the mean values for all features of all nodes can be reconstructed. The values to estimate are denoted by vector $\mathbf{y}^*$, consisting of $N$ feature-specific stacked vectors $y_i^*$ of length $M$ (one element per node). Again, contrasts are taken with the previously selected reference observations: $\Delta y_i^* = y_i^* - y_{i0}^*$. These are combined in a single contrast vector $\Delta y^* = (\Delta y_1^*, ..., \Delta y_N^*)^T$.

The desired feature values $\mathbf{y}^*$ can be estimated by finding the contrasts $\Delta y^*$ that maximize the likelihood, given the observed contrasts $\Delta y$, as well as the previously estimated phylogenetic covariances $\mathbf{a}$ and phenotypic variances $\mathbf{b}$. This likelihood is described by a multivariate normal distribution of the combined contrasts
\[ \Delta y = (\Delta y^*, \Delta y^T)^T. \] As before, the mean of this distribution equals zero, since the expectation of the two terms in any contrast is identical (namely, the corresponding feature value of the root node). The covariance matrix of the distribution can be partitioned as

\[ \Sigma = \begin{pmatrix} \Sigma^* & \Sigma^x \\ \Sigma^T & \Sigma \end{pmatrix} \]

The lower right block describes the covariances between observed contrasts, and thus equals the covariance matrix \( \Sigma \) that was derived previously. The upper left block \( \Sigma^* \) describes the covariances between the desired contrasts:

\[
\text{Cov}(y_i^* - y_{i0}, y_{jq} - y_{j0}) = a_{ij} \left( T_{pq} - T_{pm_{j0}} - T_{mj_{0q}} + T_{mj_{0m_{j0}}} \right) + \delta_{ij}b_{ij}
\]

with \( p, q \in \{1, \ldots, M\} \). It may be noted that phenotypic variability contributes at most once to the covariance: when both reference observations \((y_{i0}, y_{j0})\) are equal. It does not additionally contribute to the variance (diagonal elements of \( \Sigma^* \)) if \( y_{ip}^* \) and \( y_{iq}^* \) are equal, as desired feature values \((y_{ip}^*, y_{iq}^*)\) pertain to the nodes (the species mean), rather than to the individual samples; therefore they are not subject to phenotypic variability.

The off-diagonal block \( \Sigma^x \) and its transpose \( \Sigma^{xT} \) describe covariances between elements of \( \Delta y^* \) and elements of \( \Delta y \):

\[
\text{Cov}(y_{ip}^* - y_{i0}, y_{jq} - y_{j0}) = a_{ij} \left( T_{pm_{jq}} - T_{pm_{j0}} - T_{mj_{0q}} + T_{mj_{0m_{j0}}} \right) + \delta_{ij}b_{ij}
\]

with \( p \in \{1, \ldots, M\}, q \in \{1, \ldots, K\} \). Since these covariances describe off-diagonal elements of the combined covariance matrix \( \Sigma \) only, phenotypic variances contribute at most once to the covariance (when reference observations \( y_{i0} \) and \( y_{j0} \) are equal).

To obtain estimates for \( \Delta y^* \), the likelihood can be rephrased as the distribution of \( \Delta y^* \) conditional on \( \Delta y \). This distribution is again multivariate normal with mean \( \Sigma^* \Sigma^{-1} \Delta y \) and covariance matrix \( \Sigma^* - \Sigma^* \Sigma^{-1} \Sigma^{xT} \) (Johnson and Kotz 1972). These directly specify estimates of the desired contrasts, and their covariances. From the estimates of the contrasts the estimates for the missing feature values are easily derived by taking for each feature the sum of the estimated contrast vector and the original reference value: \( y_i^* = \Delta y_i^* + y_{i0} \). The variance of the estimates is directly equal to the diagonal of the contrast covariance matrix \( \Sigma^* - \Sigma^* \Sigma^{-1} \Sigma^{xT} \), as the reference observations act as constants in this context.

### 5.6 References


5. A generic method for estimation of trait values using phylogeny


6 Phylogeny-informed estimation of phytoplankton trait values

Submitted manuscript

Abstract
The accurate resolution of distinct phytoplankton taxa will be a key step towards improvement of current aquatic ecosystem models. With a growing interest in modelling specific taxa, however, it becomes increasingly difficult to obtain good estimates for the corresponding parameters. The present study takes an evolutionary perspective to the variability across phytoplankton taxa in order to estimate unknown parameter values. Established techniques from comparative physiology are used to integrate a new dataset with over one thousand observed freshwater phytoplankton parameters with the species phylogeny to derive robust estimates for the size, growth rate, phosphate affinity and susceptibility to predation of 277 taxa. These estimates account simultaneously for phylogenetic relationships between species, and approximate power law relationships (e.g., allometric scaling laws) between different traits as reconstructed from the dataset. Cross-validation demonstrates that the estimates significantly improve upon those provided by several alternative methods. These results could benefit most quantitative studies involving phytoplankton, and are available online at http://www.ibi.vu.nl/programs/phylopars/phytoplankton.
6. Phylogeny-informed estimation of phytoplankton trait values

6.1 Introduction

Phytoplankton serves as the base of the aquatic food web, and thus can influence every aspect of aquatic ecosystems, from the natural response to changes in nutrient loading and toxicants to commercial catches of fish. Quantitative predictions on aquatic systems on any level therefore require parameterization or explicit resolution of the role of phytoplankton. While this is generally acknowledged, aquatic ecosystem models differ considerably in the detail with which they resolve phytoplankton communities. Classic aquatic food web models (Evans and Parslow 1985; Fasham et al. 1990) describe natural systems with one phytoplankton functional type, governed by a single set of parameters that effectively comes to represent a “mean species”. This approach is still in use, and understandably popular in studies that address questions that do not pertain directly to phytoplankton. However, there are several reasons why one would consider the explicit resolution of several different phytoplankton taxa.

First, some phenomena directly involve specific phytoplankton taxa: select groups of harmful algae have the capability to severely damage populations of higher trophic levels, only specific taxa are a food source of importance for higher trophic levels, and several taxa fulfil highly specific, major roles in global elemental cycling, for instance by building silicate (diatoms) or calcium carbonate shells (coccolithophorids).

Second, even questions that do not pertain directly to phytoplankton (but for instance to zooplankton or fish) may not be answerable with a single phytoplankton functional type. Phytoplankton species display a bewildering diversity, varying in anything from energy acquisition strategy (autotrophy, mixotrophy, heterotrophy), nutrient usage (e.g., ammonium, nitrate, nitrogen fixation), defence mechanisms, and reproduction strategy (Litchman and Klausmeier 2008; Reynolds 1984; Sournia 1982). Consequently, the parameters that characterize the behaviour of a population vary substantially between phytoplankton species. Given that different species occupy distinct spatial niches and appear at different times in the successional sequence (Sommer et al. 1986), this suggests that it will be near impossible to construct a “mean” phytoplankton model that aptly captures the behaviour of a natural community in a range of temporally and spatially varying conditions. Moreover, even if such a model would successfully resolve some ecosystem properties, it is doubtful whether this can be traced back to the behaviour of the plankton the model was meant to represent – it is more likely a convenient parameterization, rather than an accurate picture of underlying processes and mechanisms. It is thus not surprising that recent aquatic ecosystem models have begun to incorporate increasing numbers of distinct phytoplankton taxa (Baretta et al. 1995; Quéré et al. 2005).
As the interest in resolving specific, narrow taxa of phytoplankton in models grows, it becomes increasingly difficult to obtain accurate, experiment-based estimates of the parameters that characterize the behaviour of each modelled taxon. An extensive amount of literature treats the identification of parameters such as maximum growth.
rates and nutrient half-saturation coefficients from laboratory experiments. These studies cover a wide range of taxa (Figure 6.1). The number of studies covering a particular taxon often correlates positively with the dominance of that taxon – for instance, the number of studies in Figure 6.1 approximately mirrors the abundance of taxa in the well-studied Lake Constance (Gaedke 1998; Sommer 1987). This might suggest that at least for some common traits, the information present in existing literature could suffice. However, this is not the case. First, there are several notable exceptions to the pattern of increased study with increased dominance: certain orders of cyanobacteria and dinoflagellates occasionally dominate the ecosystem, but have rarely been included in empirical studies. This in part relates to difficulties associated with keeping these species in culture. Second, the present dominance of taxa may not be a good predictor of their effective relevance, as rare but intense blooms of particular species can cause great and lasting changes in the ecosystem (Smayda and Reynolds 2003), and species that are currently of minor importance may take on major roles under the influence of climate change (Briand et al. 2004; Falkowski and Oliver 2007; Nehring 1998; Occhipinti-Ambrogi 2007). These species will usually not, or seldom, have been kept in culture, and therefore their parameters will be unknown. Thus, existing literature cannot provide the quantitative information needed to constrain present and future aquatic ecosystem models.

Nevertheless, the current body of knowledge on species parameters can be an important source of information as one strives to obtain a “best guess” for an unknown phytoplankton parameter. First, with a taxonomy in hand, the evolutionary closest taxon can be selected for which observations are available. Subsequently, approximate relationships between different parameters (e.g., allometric scaling laws) can be used further refine this estimate with the known value of another parameter. For instance, to estimate the maximum growth rate of a large green alga, one could take the growth rate of a related smaller species, then adjust it downward by exploiting the known approximate allometric relation between cell size and growth rate (Litchman et al. 2007; Sarthou et al. 2005; Schlesinger et al. 1981). The combined knowledge on evolutionary relationships and typical parameter correlations can permit estimation of unknown parameters. Such procedures are occasionally performed by modellers, but on an ad-hoc basis using limited information pertaining exclusively to the species and parameter at hand.

The present study demonstrates a robust, formal approach to the estimation of parameters from existing observations and evolutionary relationships. Established methods from comparative animal physiology (Felsenstein 2008; Housworth et al. 2004; Ives et al. 2007) are applied for the first time to a new, extensive dataset (>1000 values, 38 literature sources) of observed freshwater phytoplankton cell size, maximum growth rate, phosphate affinity and susceptibility to predation. From this dataset and a qualitative phylogenetic tree, the joint evolution of different traits is characterized in terms of power law relationships (e.g., allometric scaling laws) and a random noise component. Subsequently, this characterization is recombined with the phylogeny and original observations to derive best estimates for all traits and taxa in
the dataset – 1939 values in total – along with a measure of certainty. The key appeal of this method is that it permits full use of all available information: each estimated parameter value incorporates all original observations, adjusted according to power laws as well as phylogenetic proximity. Accordingly, cross-validation demonstrates that the resulting estimates improve significantly upon those obtained with several alternative methods.

This analysis can benefit modellers and experimentalists alike, both through the directly usable parameter estimates it provides, and through the associated probability distribution, usable as "prior distribution" in combination with other information in Bayesian analyses. Notably, the method allows for extrapolation to any unknown phytoplankton species: given its place in the phylogeny and (optionally) any available observation of its other traits, best estimates for all traits can be calculated. Both the existing estimates and this extrapolation functionality have been made available at http://www.ibi.vu.nl/programs/phylopars/phytoplankton.

### 6.2 Methods

#### 6.2.1 Dataset

A dataset of empirically observed phytoplankton parameters is compiled from 38 literature sources (see the appendix). The dataset is currently restricted to freshwater species, but it is part of an ongoing initiative in which marine species will be included in the future. At present, the following set of traits is included: cell length (longest axial dimension), cell diameter (shortest axial dimension), cell surface area, cell volume, maximum growth rate, phosphate affinity, and susceptibility to predation (Table 1).

<table>
<thead>
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<th>trait</th>
<th>unit</th>
<th># sources</th>
<th># species</th>
<th># observations</th>
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</thead>
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<td>49</td>
<td>59</td>
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<td>66</td>
<td>211</td>
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<tr>
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<td>29</td>
<td>49</td>
</tr>
<tr>
<td>susceptibility to predation</td>
<td>-</td>
<td>2</td>
<td>31</td>
<td>136</td>
</tr>
</tbody>
</table>

#### Size and shape

Different measures of cell size are taken from a variety of sources that includes laboratory and field observations. It may be obvious that the information in these different measures will partially overlap: length, diameter, surface area and volume
should be positively correlated. Their joint inclusion is intentional. First, it allows for a detailed representation of the cell shape, including the surface-to-volume ratio which mediates nutrient uptake (Aksnes and Egge 1991; Kooijman 2000). Second, it tests the ability of the methodology to identify correlations between traits.

**Maximum growth rate and phosphate affinity**

Phytoplankton utilizes many inorganic nutrients, notably phosphorus, nitrogen, and silicate in the case of diatoms. The present study describes only limitation by phosphate, which is effectively the controlling nutrient for most freshwater species, as anthropogenic input in freshwater systems usually ensures a nitrogen-replete environment and silicate is only used by diatoms. Accordingly, phosphate has been the focus of more limitation studies than any other inorganic nutrient.

For the dataset, results are used from controlled nutrient limitation experiments. Care is taken to include only values that meet three criteria: (1) The temperature must be kept constant at a value between 10°C and 20°C. This generally excludes the species-specific upper temperature ranges where growth decreases. (N.B. for the light intensity, a day-night cycle is permitted.) (2) Experiments must study phosphate limitation only; other resources including light must be kept at an optimal value (3) Reported parameters must have been derived with a Monod/Michaelis-Menten model, as values obtained with other models may not be comparable. An exception is made for maximum growth rates, provided the model used describes the growth rate as a monotonously increasing, saturating function of the phosphate concentration.

Affinity rather than half-saturation is used to describe the effect of phosphate limitation. This choice was made because, unlike the half-saturation, affinity is directly associated with the processes involved in nutrient uptake, e.g., with the number of transporters per unit surface area (Aksnes and Egge 1991). It equals the ratio of the maximum growth rate to the half-saturation coefficient, which formally defines it as the biochemical affinity scaled to the biomass-on-nutrient yield.

Both maximum growth rates and nutrient affinities are standardized to continuous illumination and a temperature of 20°C. To adjust for experimental light periods of less than 24 hours, rates are multiplied with the ratio between 24 and the original light period in hours. To adjust for different temperatures, a $Q_{10}$ relationship with factor 1.88 is applied (Eppley 1972; Schlesinger et al. 1981). More detailed formulations of the temperature dependence, such as Arrhenius- or activation-deactivation kinetics (Sharpe and Demichele 1977), parameterized by the observed maximum growth rates in the dataset, did not noticeably improve results. This may relate to the fact that different taxa have very different temperature-response curves, and to the fact that we consider only a narrow range of temperatures (10°C – 20°C) in which a reduction of growth due to high temperature typically does not occur.
Susceptibility to predation

The susceptibility to predation of a prey species is by definition specific to the predator species, which can vary from mixotrophic and heterotrophic nanoplanckton to crustaceans (daphnids, *Cyclops*, *Eudiaptomus*), bivalves and other organisms. The present study exclusively considers predation by daphnids, for two reasons: first, daphnids are among the best studied algal predators, and second, results of the present work will be used to describe succession in Lake Constance (Bruggeman et al., in prep.) where daphnids are dominant predators (Sommer 1987).

Susceptibility to predation is defined with respect to *Daphnia* sp. In the literature sources used, susceptibilities are reported with respect to the species *D. hyalina*, *D. galeata*, *D. longispina*, and *D. magna*. The susceptibility itself is generally reported as the rate of prey consumption (fraction of the population per unit time), relative to the rate at which the (locally) favourite prey is consumed (Vanderploeg and Scavia 1979).

To standardize these values across experiments, the values are re-normalized to the local relative consumption of a single prey species, *Rhodomonas minuta*. This species is chosen because its rate of consumption is reported in most experiments included in the dataset. For those studies not involving *Rhodomonas*, its potential consumption is estimated by multiplying the reported consumption of another species to the typical ratio in consumption between *Rhodomonas* and that species; this ratio is derived from the other experiments. Thus susceptibility to predation comes to represent the rate of consumption by *Daphnia* sp., relative to its consumption of *Rhodomonas minuta*.

6.2.2 Modelling evolution

In order to estimate unknown parameters, the relationships between these and existing observations must be made explicit. To relate all phytoplankton parameters, they are interpreted as the outcome of the evolution from a single primordial phytoplankton species, with repeated branching having given rise to the present day species. In turn, each observation in the dataset is then taken to be a sample of an unknown, evolution-shaped species mean.

Random walks

In the absence of detailed information on the direction of natural selection, the neutral model for the evolution of continuous traits is that of genetic drift: on evolutionary time scales species perform a random walk in trait space. This is also called the “Brownian motion” model of evolution (Felsenstein 1988), which states that after a given period of time very many, very small, independent random changes in the trait value have occurred. Since these changes are random, there is no selection in favour of either low or high values: the trait value is as likely to increase as it is to decrease. Brownian motion is formally described by a Wiener process, which has the feature that the likelihood of observing a particular trait value after a time period is given by a normal distribution. The mean of this distribution equals the trait value at the start of the random walk, since there is no selection in any direction. The variance of the distribution is proportional to the length of the period: after a longer time period, a
larger number of random steps has been taken, so there is a larger change of observing trait values that differ considerably from that of the ancestor. The coefficient of proportionality can be through of as a measure of the distance travelled in a random step, and thus specifies the rate of evolution; this coefficient has been termed the “phylogenetic variance” (Felsenstein 2008).

Extension to multiple traits is straightforward, and introduces an interesting feature: random steps are now taken simultaneously in multiple dimensions (one dimension per trait). While successive steps are independent, the directions taken in the individual dimensions (cell volume, maximum growth rate, susceptibility to predation, etc.) in a single step need not be. Thus the changes in different traits may be correlated, e.g., an evolutionary change in cell size could correlate negatively with the change in maximum growth rate. Analogous to the univariate case, the likelihood of observing a particular set of trait values after a given period is described by a multivariate normal distribution. The mean of this distribution equals the set of ancestor trait values, and its variances and covariances can be written as the product of evolutionary time and “phylogenetic” covariances (Felsenstein 1985; Felsenstein 2008). The phylogenetic covariances can be rephrased in terms of phylogenetic regression coefficients (Garland and Ives 2000) – the ratio of a covariance and a variance for the two-trait case – describing the slope of the average trend that would emerge if changes in different traits were plotted against each other.

Introducing the phylogeny

A phylogenetic tree connects species and their ancestors with branches that represent evolutionary time periods. In the context of the random walk model, each branch can be viewed as a period in which a random walk in trait space took place. For the sake of simplicity, it is commonly assumed that the same random walk process underlies all evolutionary changes, i.e., a single set of evolutionary rates and correlations applies to the complete phylogeny (Felsenstein 2008; Ives et al. 2007; Lynch 1991). This assumption becomes increasingly suspicious as one considers more widely diverged species, but is necessary as observations generally do not provide sufficient information to constrain variable evolutionary rates and correlations (Felsenstein 1988; Felsenstein 2008). The evolutionary process is thus described by a single set of “phylogenetic” covariances.

For each species, the likelihood that it has a certain set of trait values can now be represented as a multivariate normal distribution, with its mean equal to the trait values of the root of the tree, and its covariances proportional to the distance between the species and the root. If we compare trait values of two different species, it is evident that these have evolved independently only since their evolutionary lineages branched from their last common ancestor. Unless this ancestor is the root of the tree, their trait values are consequently correlated. The strength of this correlation is determined by the length of their shared evolutionary path (from root to common ancestor), relative to that of their total evolutionary path (from root to species)
(Felsenstein 1985). Both are defined by the evolutionary model in terms of phylogenetic covariances. Together these properties completely specify the multivariate normal likelihood of observing any subset of parameters across all taxa.

**Power law relationships**

The use of a single set of phylogenetic covariances throughout evolution is equivalent to assuming that the same linear model underlies all evolutionary change. This implies that the slope of the regression of one trait on another is constant. Relationships between phytoplankton traits may be better approximated by (multivariate) power laws rather than linear relationships, as earlier studies have proposed that phytoplankton traits are governed by allometric laws (Litchman et al. 2007; Sarthou et al. 2005; Schlesinger et al. 1981). Therefore, the natural logarithm is taken of all observed parameters [equivalently, this assumes that relative changes in trait value are well described by a zero-mean random process], thus imposing power law relationships between parameters, rather than linear ones. This allows the evolutionary model to capture commonly proposed allometric relationships among traits.

The log transformation of parameter values makes power law relationships govern each individual evolutionary change. It should be noted, however, that these relationships do not necessarily equal those obtained by simple regression of one trait on another, when these are based upon observations across species without regard for phylogenetic relationships (Litchman et al. 2007; Sarthou et al. 2005; Schlesinger et al. 1981). Felsenstein (1985) demonstrated with simulations that such non-phylogenetic analyses easily overestimate the significance of correlations between traits, or even perceive relationships when the underlying mechanism lacks these.

**Phenotypic variability**

The phylogenetic model is extended to account for “phenotypic” variability (Felsenstein 2008), which includes measurement error and intraspecific variation. This is an essential addition for many purposes, as the observed variability in trait values is often for a significant part due to measurement error (Ives et al. 2007). Phenotypic variability is assumed to be described by a normal distribution centred at the phylogenetic mean of the trait. This distribution has a certain trait-specific “phenotypic” variance which characterizes phenotypic variability. Correlation between observed trait values is assumed to be due exclusively to evolutionary processes (and not to the measurement process itself), eliminating the need to consider phenotypic correlations (cf. Felsenstein 2008). Effectively, phenotypic variability acts like an extension of the evolutionary path: it adds a layer of variability below between the species’ expected value and the observation. As a result, the likelihood of observing a certain set of trait values remains multivariate normal: the variances of the phylogenetic and phenotypic models are simply summed to arrive at sample variances (covariances remain unaffected, which implies that phylogenetic variability reduces the correlation between observations).
Constructing a phytoplankton phylogeny

The accuracy of the predictions of the evolutionary model is to a large extent determined by the quality of the phylogeny in terms of topology and branch lengths. Phylogenetic branch lengths ideally represent evolutionary time, which is a reasonable assumption only for recent phylogenies based on gene or protein similarity. To our knowledge, however, there does not exist a complete phylogeny based on molecular evidence that spans all eight phyla of “phytoplankton” present in the dataset. Therefore, a recent taxonomy (Guiry and Guiry 2009, http://www.algaebase.org), supplemented with up-to-date information on the evolution of higher taxonomic ranks (Maddison and Schulz 2007, http://tolweb.org), is used as surrogate for the evolutionary tree. Distances between consecutive taxonomic ranks (domain-kingdom-phylum-class-order-family-genus-species-variation) are arbitrarily taken equal (cf. Cheverud et al. 1985). This is certainly a crude approximation of the true phytoplankton phylogeny, but it has previously been demonstrated that even an analysis with this type of qualitative phylogeny is to be preferred over nonphylogenetic approaches (Martins and Garland 1991).

Predicting parameter values

The final model specifies that the likelihood of observing any set of trait values for any set of species is given by a multivariate normal distribution. The mean of this distribution equals the set of (unknown) trait values of the root of the phylogenetic tree. The covariances of the distribution depend on the tree topology and branch lengths, as well as the unknown phylogenetic covariances and phenotypic variances. One can attempt to estimate these by maximizing the likelihood of observing the phytoplankton dataset. To start, the problem can be simplified by eliminating the dependency on the root trait values (Felsenstein 2008; Ives et al. 2007; Revell and Harmon 2008). However, the covariances between observations still depend on phylogenetic and phenotypic covariances in such a way that analytic estimation of these parameters is impossible. Therefore, the likelihood is maximized numerically, using a recently introduced approach that accounts for phylogenetic and phenotypic variability, and additionally permits missing data (Bruggeman et al. 2009, http://www.ibi.vu.nl/programs/phylopars).

Given best estimates for the model’s phylogenetic and phenotypic covariances, it is straightforward to define the likelihood of finding both the known (observed) and the unknown (desired) parameters as yet another multivariate normal distribution, in which only the expectation of the unknown parameters is unknown (Bruggeman et al. 2009). The best estimate for the unknown parameters can thus be found by calculating the expected value of a multivariate normal distribution, conditional on the observed parameter values. In similar fashion, the covariances of these estimates can be calculated. Both calculations are straightforward (Johnson and Kotz 1972).
6.2.3 Validation

The quality of the parameter estimates is investigated through cross-validation: observations are one by one omitted from the dataset, then re-estimated with the evolutionary model. This produces an estimation difference for each original observation. From these differences the mean absolute error (the mean of the absolute differences) is calculated, which serves as indication of the expected accuracy for estimates of unknown trait values.

The present model integrates two concepts: (A) “relations between taxa” – phylogenetically related species will have similar parameters, (B) “relations between traits” – changes in different traits may be correlated and approximated with power laws. To investigate the independent influence of these two components, cross-validation statistics are also calculated with these two components removed from the model. To eliminate the influence of the phylogeny, the analysis is performed with the original phylogenetic tree replaced with a dummy phylogeny with star topology (Garland et al. 2005). This topology describes the scenario where all species evolved independently from one single common ancestor, causing the phylogeny to resemble a star. To eliminate the correlations between the different traits, the analysis is performed as before, but with all phylogenetic correlations set to zero instead of being estimated from the dataset. It is worth noting that when both components are removed, the model effectively becomes a “mean model” (Bruggeman et al. 2009) that takes the mean value of a given trait as the best estimate for all taxa.
6. Phylogeny-informed estimation of phytoplankton trait values

6.3 Results

Figure 6.2. Relative cross-validation errors with and without relationships between taxa and traits. These error measures equal the exponential of the mean absolute error (defined in the natural logarithm of the trait units, since all traits are log-transformed), with 1 subtracted – this is identical to the geometric mean of relative estimation errors. Results are presented for a non-phylogenetic model (using a phylogeny with star topology) without power law relationships between traits, for the model with only power law relationships, for the model with only the phylogeny, and for the full model with both the phylogeny and power laws.

6.3.1 Validation

A compact overview of the typical accuracy of the estimated trait values is given by the cross-validation errors shown in Figure 6.2. Results are presented for four analyses: with neither phylogenetic relationships between phytoplankton species nor power law relationships between traits (mean model), with power law relationships only, with phylogenetic relationships only, and with both phylogenetic relationships and power law relationships (the full model). By comparing the different estimation errors, one can judge the improvement due to assumptions of “relations between species” and “relations between traits”. Particularly, the improvement due to the incorporation of phylogenetic relationships between species can be interpreted as an indication of the heritability of the different traits.
It is clear that the joint representation of relationships between taxa and traits allows for considerable improvement in parameter estimates (black bars vs. white bars): the error reduction varies between a factor 1.2 (susceptibility to predation) and 15 (surface area), with a typical error reduction of a factor two. Moreover, it is clear that the inclusion of the phylogeny alone substantially reduces estimation errors in most cases (light-grey bars vs. white bars; black bars vs. dark-grey bars): errors in cell volume, length, maximum growth rate and phosphate affinity are reduced by average factors 2.4, 1.4, 1.6 and 1.5, respectively. An exception to this pattern can be seen for the cell diameter and susceptibility to predation – for these traits the inclusion of the phylogeny bring a negligible improvement in estimates.

### 6.3.2 Parameter estimates

Space limitations preclude a complete listing of the estimates for all 7 traits of all 277 taxa. Instead, estimates have been made available at [http://www.ibi.vu.nl/programs/phylopars/phytoplankton](http://www.ibi.vu.nl/programs/phylopars/phytoplankton). This online resource contains estimated trait values as well as their standard errors, confidence intervals, and probability distribution.

Figure 6.3 shows the predicted values for a subset of traits: the cell volume, maximum growth rate and susceptibility to predation. These have been selected to provide insight in the role of cell size, and in the balance between bottom-up and top-down controls. Predictions are visualized as a phylogenetic tree with the parameter values gradually evolving from a single common ancestor to the individual phytoplankton families. Each individual taxon is coloured according to the parameter predicted by the evolutionary model, and colour gradients indicate evolutionary change.

The figure suggests that taxonomic grouping of trait values occurs for all three selected traits: particularly on the class level (each second branch point when seen from the right) trait values are conserved. Particular groups of phytoplankton do stand out from their phylogenetic neighbours: diatoms (Achnathaceae, Bacillariaceae, Coscinodiscaceae, Fragilariaceae) have notably high maximum growth rates, cryptophytes (Pyrenomonadaceae, Chroomonadaceae, Cryptomonadaceae) have high growth rates and a very high susceptibility to predation, and dinoflagellates (Gymnodiniaceae, Peridiniaceae, Ceratiaceae) are large, have low growth rates and low susceptibility to predation.

Additionally it can be observed that the cell volume correlates negatively with both others traits: the maximum growth rate and susceptibility to predation tentatively display a trend that is opposite (high to low values when seen from top to bottom) to the trend in cell volume (from low to high), particularly within orders and between families, and within phyla between classes. This is confirmed by the estimates for the phylogenetic regression coefficients: these differ significantly from zero, equalling \(-0.20\) for the logarithm of the maximum growth rate and \(-0.26\) for the logarithm of the susceptibility to predation, both regressed individually on the logarithm of cell volume.
6. Phylogeny

Phytoplankton trait values estimation of phytoplankton trait values

- cell volume
- maximum growth rate
- susceptibility to predation
6.4 Discussion

6.4.1 Accuracy and uncertainty

By explicitly taking phylogenetic relationships between species and correlations between traits into account, the present analysis substantially improves estimates of phytoplankton parameters: relative estimate errors are reduced with a factor two on average, compared to those obtained with a non-phylogenetic analysis unaware of correlations between traits. Yet there is no avoiding the fact that phytoplankton parameters display great inter- and intraspecific variability. The relative error in the maximum growth rate is still 37% at minimum, and for the susceptibility to predation and the phosphate affinity the minimum error remains at 96% and 157%, respectively. A key feature of the analysis is therefore that it quantifies the remaining uncertainty: in addition to point estimates, the method provides standard errors, confidence intervals and a probability distribution for each of its estimates. Applications that utilize these results would be well advised to take these uncertainties into consideration. Ideally, they would incorporate further empirical information. The probability distribution or confidence intervals provided by the present method could then serve as constraint for Bayesian or classic constrained parameter estimation, respectively.

6.4.2 Heritability

Phytoplankton communities may be better characterized by the presence and absence of certain functional types, rather than specific taxa (Quéré et al. 2005; Reynolds et al. 2002). Functional types have been suggested to be polyphyletic, i.e., species from different taxa perform similar roles (Reynolds et al. 2002). Given the variability within taxa and the similarities across taxa, can the phylogeny actually contribute to the estimation of the functional traits of a species? The present results indicate that for certain traits, this is certainly the case.

For nearly all traits included in this study, the explicit representation of phylogenetic relationships brings a considerable improvement in the accuracy of trait value estimates. The relative error in estimated cell volume is reduced by factor 2.4, the error in maximum growth rate by a factor 1.6, and the error in phosphate affinity by a factor 1.5 (Figure 6.2). These error reductions indicate that these traits are heritable:
similar species can only have similar values if the traits are conserved in evolution. For the cell volume that is not very surprising; related species often have similar sizes. Instead it is rather surprising that the cell diameter displays no heritability, which may relate to the fact that the diameter shows little variability in the first place. More importantly, this study demonstrates that physiological characteristics of phytoplankton are heritable: the maximum growth rate and phosphate affinity are to certain extent conserved in evolution. Results quantitatively support the commonly held view that diatoms as a group have notable high growth rates, whereas dinoflagellates as a group have low ones (Quéré et al. 2005; Varela et al. 1995): the ancestral diatom has an estimated maximum growth rate of 1.4 /d vs. 1.0 /d for its ancestor, the heterokonts, while Dinophyceae grow with 0.47 /d vs. 0.98 /d for the Chromalveolata (Figure 6.3). In contrast to physiology-related traits, the susceptibility to predation shows negligible heritability. This may result from the fact that the susceptibility is a complex trait which is unlikely to have a simple genetic basis. The fact that this type of trait shows little heritability agrees with the notion that behavioural and ecological traits show less phylogenetic signal than physiological traits (Blomberg et al. 2003).

6.4.3 Merits of the evolutionary model

The present Brownian motion evolutionary model is the simplest conceptual model that could be used to describe the variability in continuous traits across taxa: it uses a linear model to describe the correlation between different traits, and ascribes all further variability to neutral (i.e., zero-centred) random processes. This contrasts notably with recent attempts to describe evolution of plankton under the influence of directional natural selection by intrinsic and extrinsic factors (Jiang et al. 2005; Litchman et al. 2009; Verdy et al. 2009). It might seem tempting to apply that type of detailed analysis to the evolution of all phytoplankton taxa within the present study. However, this requires an holistic approach in which not only the variable abiotic and biotic environment, but also the physiology of all taxa and their co-occurrence in all different environments is modelled explicitly. Given our limited qualitative knowledge on past aquatic environments, and a definite lack of quantitative information, such an effort is clearly not feasible. Fortunately, the Brownian motion model has certain favourable characteristics despite of (or perhaps thanks to) its simplicity. It has been shown that the resulting mathematical description can be motivated on first-principle statistical grounds, independent of the specific assumptions of the Brownian motion model (Garland and Ives 2000; Grafen 1989). Accordingly, its predictions have been shown to be robust even if certain model assumptions are violated (Martins et al. 2002). In the absence of detailed information on evolutionary processes, the Brownian motion model provides a robust base model for the present analysis.

Within the context of the Brownian motion evolutionary model, the accuracy of the parameter estimates depends in part on the quality of the phylogenetic tree: both the tree topology and branch lengths directly feature in the result. Ideally the tree is derived from independent, detailed information, e.g., gene or protein similarities.
However, this is at present not possible for the "nineteenth century ecological construct for a biologically diverse group of pelagic photoautotrophs" (Quigg et al. 2003) that is phytoplankton: the present dataset alone contains species from eight phyla. The present phytoplankton phylogeny is therefore based on taxonomic classifications. Taxonomy-based phylogenies contain considerable more polytomies (one ancestor species branching into more than two descendant species) than expected for evolutionary trees, and use arbitrary distances between taxonomic ranks (Garland et al. 2005). Thus, the true phytoplankton phylogeny would likely be considerably different. In view of this, the considerable improvement in trait value estimates if the present qualitative phylogeny is used (Figure 6.2) is reassuring. It suggests that the current taxonomy-based phylogeny does capture the dominant relationships between species.

6.5 Conclusion

The present method uses a phytoplankton phylogeny to obtain an evolutionary reconstruction of past and present phytoplankton parameters. Cross-validation demonstrates that the resulting estimates are typically a factor two more accurate than those obtained with alternative methods. The method provides point estimates for 7 traits of 277 taxa (summarized for phytoplankton families and higher taxonomic ranks in Figure 6.3), along with standard errors, confidence intervals and probability distributions. By offering details for all taxa online, in combination with a facility to derive estimates for species not in the dataset, this study could contribute to most quantitative studies involving phytoplankton.

6.6 References


6.7 Appendix: literature sources


6. Phylogeny-informed estimation of phytoplankton trait values


Summary

This thesis addresses the general problem of describing complex natural communities with models that are necessarily simple. The work is inspired by marine plankton communities, whose influence on the global climate is large but dependent on their species composition. First, a conceptual framework for community modelling is developed, which is defined in terms of the distribution of key properties – traits – within the community. Communities are then allowed to self-assemble through competition among a large collection of virtual species, differing only in the value of one or more traits. Subsequently, a mathematical approximation is developed that reduces these large collections of species to a few key statistics, which can then be simulated with good computational efficiency. To do justice to the substantial spatial and temporal variability in the marine environment, model communities are embedded within a realistic, spatially-explicit representation of the marine water column. The resulting spatiotemporal variability allows the community models to reproduce a variety of observed patterns in aquatic systems. Finally, the abstract concept of traits is connected to actual observations: an evolution-based approach is used to identify dominant traits and trade-offs from sparse observations on natural species. These patterns in interspecific differences can directly inspire and constrain future trait-based community models.

Chapter 2 introduces a high-level conceptual approach to community modelling. This approach focuses on dominant interspecific differences (traits and trade-offs) and functional diversity, rather than on the specific properties of individual species. All species are modelled with a qualitatively identical model, and differ only in their value of one or more continuous traits. The state of the community is described by the distribution of biomass over all possible trait values. In a spatially and temporally varying environment, the dynamic behaviour of the community is then completely represented by changes in the shape of the trait distribution. This conceptual approach is tested with a simple, four-parameter phytoplankton model with two traits: the investment in light harvesting and the investment in nutrient harvesting. The distribution of these traits is modelled by discretizing both trait axes, rendering hundreds of virtual phytoplankton species that differ in light- and nutrient harvesting capability. This community model is embedded within a one-dimensional model of a turbulent water column, which explicitly resolves temporal and spatial variability in light and nutrient fields. In this setting, the model captures several well-known aquatic ecosystem features, including formation of a deep chlorophyll maximum and nutrient-driven seasonal succession.

Chapter 3 extends the conceptual, distribution-based framework by introducing a method for aggregating large numbers of virtual species. It starts with a community of species, modelled as a probability distribution of one or more continuous traits. This
distribution is then characterized by a few key statistics: the distributional moments. The reduction to these statistics preserves key aspects of the community structure, such as the typical properties of the species (the mean of the traits) and a measure of functional diversity (the variance of the traits). Instead of discretizing the trait distribution, as in chapter 2, it is now modelled by describing the dynamics of its lower moments. Spatial variability is explicitly considered: the derivation investigates the scenario where the community is transported by advection and diffusion in spatially-explicit hydrodynamic models. This turns out to pose specific requirements on the statistics that can be used to characterize the trait distribution. The final result is an approximation of community dynamics in terms of a limited number of variables. This approximation is computationally very efficient, allowing the use of this type of community model in the spatially structured environments created by one-dimensional and three-dimensional hydrodynamic models.

Chapter 4 demonstrates the capabilities of the aggregation method, by applying it to a plankton community with two traits: the investment in autotrophy and the investment in heterotrophy. This could be considered the smallest possible self-sustaining community: autotrophic machinery forms organic matter from inorganic nutrients and energy provided by light, and heterotrophic machinery breaks down organic matter into inorganic nutrients. The community structure is represented by the distribution of biomass of all possible combinations of autotrophic and heterotrophic investments. This representation is particularly appealing because it permits the existence of mixotrophs that combine autotrophic and heterotrophic feeding modes; these mixotrophs are believed to fulfil key roles in nature. The bivariate trait distribution is reduced to the total biomass, mean autotrophic and heterotrophic investments, and covariances of these investments. This renders a minimal model that does a surprisingly good job at reproducing known spatiotemporal patterns in chlorophyll, mixotrophy and phytoplankton diversity. Moreover, additional simulations with a discretized trait distribution demonstrate that the approximation in terms of distributional moments performs well: quantitative discrepancies for the total biomass and mean investments are low, while covariances show good qualitative correspondence. This indicates that it is possible to derive distribution-based community models that deliver accurate representations of natural systems without requiring a large computational effort.

Distribution-based community models suffer from an important practical problem: it is difficult to pinpoint which traits dominate interspecific differences in reality, and how these traits affect organism behaviour. To tackle this problem, chapter 5 discusses how the sparse observations can be used to estimate the trait values for any species. This is based upon a simple evolutionary model that represents the evolution of multiple traits as a correlated random walk from a single primordial species. From a set of observed trait values and the species phylogeny, the model reconstructs both the rate of evolution and the trade-offs between different traits. This information is then recombined with the original observations to produce trait value estimates for all taxa in the phylogeny.
Chapter 6 demonstrates the feasibility of the evolution-based approach to reconstructing traits and trade-offs of chapter 5 by applying it to a new, extensive database of observed phytoplankton trait values. This database comprises 7 different traits, including cell size, maximum growth rate, nutrient affinity and susceptibility to predation, and 277 phytoplankton taxa. From a limited number of observations, the method calculates point estimates for all traits of all taxa (1939 values), along with standard errors, confidence intervals and probability distributions. These estimates provide valuable information on the traits and trade-offs that dominate interspecific differences in real phytoplankton communities. Moreover, in providing estimates for a variety of traits and species, these results can contribute to most quantitative studies involving phytoplankton.

In conclusion, this thesis provides conceptual and mathematical building blocks for models that target the macroscopic behaviour of the community, rather than the details of individual species. By combining methods for the identification of traits and trade-offs, the process-based formulation of trait-based models, the reduction of complex communities to a few key statistics, and the embedding of such reduced models in a spatially explicit context, natural systems can be modelled without necessitating extreme model complexity. Application to marine plankton communities demonstrates that this produces models that maintain computational efficiency while reproducing a wealth of features of natural ecosystems.
Samenvatting

Introductie
De soortsamenstelling van ecosystemen bepaalt hoe de natuur functioneert en reageert op verandering. Wanneer we het gedrag van een ecosysteem willen voorspellen, is het dan ook aantrekkelijk om het systeem op te vatten als de som der delen: eerst karakteriseren we het gedrag van iedere individuele soort, en daarna combineren we deze soortbeschrijvingen in een modellecosysteem. Onze kennis over individuele soorten schiet echter vrijwel altijd tekort voor deze aanpak.

Dit proefschrift richt zich daarom juist op de overeenkomsten tussen soorten: een beschrijving van een algemene, “alleskunnende” populatie dient als basis voor alle soorten in het ecosysteem. Verschillen tussen soorten worden aangetoond door de waarden van bepaalde soorteigenschappen (“traits”) te variëren. Soorten verschillen dus enkel kwantitatief, in de mate waarin ze deze eigenschappen tentoonspreiden; de manier waarop ze functioneren is gelijk.

Vervolgens laten we het ecosysteem zichzelf organiseren volgens het principe “alles is overal, het milieu selecteert”: grote aantallen verschillende soorten worden gezamenlijk blootgesteld aan een realistische omgeving. Doordat de eigenschappen van sommige soorten beter aansluiten bij de omgeving zullen ze andere eruit concurreren, waardoor een specifieke soortsamenstelling ontstaat. Onder invloed van de seizoenen verandert de omgeving voortdurend en daarmee zijn op ieder moment weer andere soorteigenschappen optimaal. Daardoor blijft de soortsamenstelling van het ecosysteem continu veranderen. Het aardige van deze aanpak is dat het met een klein aantal simpele regels toch mogelijk wordt om structuur en diversiteit van levensgemeenschappen te beschrijven. Dit is ideaal om te bestuderen hoe deze gemeenschappen zich aanpassen aan een veranderende omgeving (bv. onder invloed van klimaatverandering).

Deze ideeën worden in dit proefschrift uitgewerkt tot een volledig raamwerk voor het beschrijven van ecosystemen in termen van soorteigenschappen. Dit wordt geïllustreerd met een toepassing voor plankton in de oceaan: met twee eigenschappen blijkt het al mogelijk om diverse patronen in de soortsamenstelling van plankton in tijd en ruimte te reproduceren. Dit opent de weg voor toepassing op grotere natuurlijke systemen en voor vergelijking met observaties.

Aanleiding: de biologische koolstofpomp
Dit onderzoek komt voort uit de noodzaak om de relatie tussen mariene ecosystemen en het broeikasgas CO₂ te kwantificeren. Aan het oppervlak van de oceanen legt eencellig fytoplankton CO₂ vast in nieuwe biomassa door fotosynthese. Het fytoplankton dient als voedsel voor klein zoöplankton, wat op haar beurt weer groter zoöplankton en vis voedt. Bij het pad dat de vastgelegde koolstof aflegt door het
voedselweb kan op verschillende punten een fractie wegzinken naar de diepzees. Dit gebeurd in het bijzonder door het zinken van de individuele cellen van sommige soorten fytoplankton en de feces van sommige soorten zoöplankton. Daarmee is het wegzinken direct afhankelijk van de soortsamenstelling van de planktongemeenschap. Door het wegzinken wordt koolstof effectief getransporteerd van de atmosfeer naar de diepzees. Dit proces wordt daarom ook wel de biologische koolstofpomp genoemd.

Dankzij de biologische koolstofpomp is de concentratie van CO₂ in de atmosfeer momenteel lager dan te verwachten zou zijn op grond van enkel fysische principes. Het is echter onzeker hoe de biologische pomp zal reageren op de huidige klimaatverandering. Voor de ecosystemen aan de oppervlakte van de oceaan heeft klimaatverandering drie directe consequenties: de temperatuur neemt toe, de menging neemt af (en daarmee de communicatie tussen oppervlak en diepzee), en het water verzuurt. Het is zeker dat deze veranderingen invloed zullen hebben op het mariene ecosysteem en daarmee op de werking van de biologische koolstofpomp, maar het precieze effect is onbekend. Het is zelfs onzeker of deze aanstaande veranderingen de pomp zullen verzwakken of versterken! Om dit in te kunnen schatten is een kwantitatieve beschrijving van het mariene ecosysteem nodig die recht doet aan de soortsamenstelling van de planktongemeenschap.

Modellen
Een kwantitatieve beschrijving van een natuurlijk systeem vereist het gebruik van modellen: beschrijvingen van het gedrag van het systeem in termen van wiskundige vergelijkingen. In het meest simpele geval is hierbij te denken aan een beschrijving van het verloop van een natuurlijke populatie als een combinatie van een reproductie- en sterftekans, beide uitgedrukt in aantal individuen per tijdseenheid. Dit zou een simpel model opleveren met twee constante termen (positief voor reproductie, negatief voor sterfte) die samen de nettopopulatiegroei vastleggen. Het verhaal wordt ingewikkelder wanneer de reproductie en sterfte afhankelijk van omgevingsfactoren, van de grootte van de populatie, of van de aanwezigheid van andere soorten (bv. predatoren). De kunst van het maken van modellen ligt in het identificeren van alle factoren die een rol spelen in het gedrag van het systeem en het definiëren van de precieze wiskundige relaties tussen deze factoren en het systeem. Dat laatste gebeurt idealtier op basis van kennis over de mechanismen die voor de relatie verantwoordelijk zijn.

Wanneer het model wiskundig is gedefinieerd, is het verhaal nog niet compleet. Een model bevat gewoonlijk diverse constante termen, “parameters”, die verschillende aspecten van het systeem vastleggen. Deze parameters omvatten bijvoorbeeld de maximale groeislag van een populatie, de onderhoudskosten van biomassa, of de aanwezigheid van de populatie voor verschillende nutriënten. De waarden van deze parameters dienen ingevuld te worden voordat het model kan worden gebruikt voor voorspellingen. Het bepalen van parameterwaarden gebeurt idealiter op basis van onze kennis van het echte natuurlijke systeem, op basis van observaties uit het
laboratorium of het veld. Deze observaties zijn helaas maar zelden toereikend om alle parameters van een model volledig vast te leggen. Dit kan komen doordat het model parameters bevat die per definitie moeilijk meetbaar zijn, of doordat de gemodelleerde soorten maar moeilijk te observeren zijn. Hierdoor ligt iedere parameterwaarde in een model nooit volledig vast en zijn modelvoorspellingen geassocieerd met een mate van onzekerheid, zelfs als de modelleur in staat geweest zou zijn om alle natuurlijke relaties volledig in zijn model te verwerken. Vaak kan de betrouwbaarheid van een model daarom verbeterd worden door minder detail (en parameters) op te nemen in het model, zodat de observaties de waarden van de overgebleven parameters preciezer kunnen vastleggen: modelleren is ook de kunst van het weglaten.

**Traditionele mariene ecosysteem modellen**

De huidige modellen van planktonsystemen zijn traditiegetrouw gebaseerd op het concept "functionele groepen": iedere groep van soorten waarvan men vermoedt dat die een unieke rol vervuld in de natuur wordt als aparte variabele opgenomen in het model. Dit begon met de nutrient-fytoplankton-zoöplankton (NPZ) en nutrient-fytoplankton-zoöplankton-detritus (NPZD) modellen eind jaren tachtig. Deze modellen waren met drie of vier variabelen relatief eenvoudig en namen nagenoeg geen enkel aspect van de soortsamenstelling mee in hun beschrijving van het ecosysteem. Desalniettemin waren ze bijzonder succesvol in het reproduceren van kenmerkende "grove" patronen in planktongemeenschappen, bijvoorbeeld het moment waarop de lentebloei in fytoplankton aanvangt.

In latere jaren werd het meer en meer duidelijk dat plankton een enorme functionele diversiteit kent: verschillende soorten vervullen heel verschillende functies in het ecosysteem. Dit leidde diverse wetenschappers ertoe om de oorspronkelijke groepen fytoplankton en zooplankton onder te verdelen in een aantal kleinere functionele groepen op basis van hun unieke functie in de natuur. De resulterende modellen omvatten tientallen variabelen en honderden parameters. Deze modellen bieden duidelijk een betere afspiegeling van natuurlijke planktongemeenschappen dan de klassieke NPZ(D) modellen. Het zou dan ook voor de hand liggen dat ze daarmee betrouwbare voorspellingen kunnen leveren, maar dit is niet noodzakelijk wederwijze het geval. De grote aantallen parameters in deze modellen worden bij lange na niet vastgelegd door de beperkte laboratorium- en veldobservaties die voorhanden zijn. Hierdoor zijn de waarden van de parameters in deze modellen zeer onzeker, en de modelvoorspellingen ook. Ironisch genoeg zijn de klassieke NPZ(D) modellen op dit moment nog het meest betrouwbaar en het meest gebruikt. Het mag echter duidelijk zijn dat deze modellen nauwelijks inzicht bieden in de structuur van planktongemeenschappen. Daarmee kunnen ze geen antwoord geven op vragen waarbij de soortsamenstelling van het ecosysteem een rol speelt, zoals het functioneren van de biologische koolstofpomp.
De soortsamenstelling bepaalt voor een belangrijk deel het gedrag van natuurlijke systemen, maar het lijkt onmogelijk om realistische soortdiversiteit toe te voegen aan modellen zonder deze te overladen met onzekerheden. Toch is dit het probleem wat dit proefschrift aankijkt: door een alternatieve benadering voor het modelleren van gemeenschappen worden het mogelijk om met minimale complexiteit toch een indicatie te krijgen van (veranderingen in) de soortsamenstelling.

**Inspiratie**

De inspiratie voor de werk komt deels van de "Adaptive Dynamics" (AD) methode voor het modelleren van evolutie, waarin een belangrijke rol is weggelegd voor zelforganisatie van het systeem door competitie tussen soorten. De AD methode gaat uit van een aanwezige populatie, de "resident", wiens nakomelingen imperfecte kopieën zijn: deze verschillen licht in een of meer geselecteerde eigenschappen. Als een nakomeling ("mutant") verschijnt wiens eigenschappen beter aansluiten bij de huidige omgeving, dan zal deze de ouder eruit concurreren, en de rol van de "resident" overnemen. Evolutie kan zo worden samengevat als de verandering van de waarde van de geselecteerde soorteigenschappen. Het intrigerende van deze methode is dat een relatief simpel model gecombineerd met willekeurige variatie in een beperkt aantal parameters, rijk en realistisch gedrag kan vertonen zonder dat er enorme complexiteit (en grote aantallen parameters) noodzakelijk zijn. In dit proefschrift worden deze concepten overgeplaatst van evolutionaire tijdsschalen naar ecologische tijdschalen.

Een belangrijke andere bron van inspiratie is de Dynamische Energy Budget (DEB) theorie. Deze theorie beschrijft de stromen van energie en massa door natuurlijke systemen, zoals individuele organismen en populaties. De nadruk ligt op de formulering van één enkele goedgefundeeerde modelstructuur die kan worden toegepast op alle levende organismen, van bacteriën tot walvissen. Verschillen tussen soorten zijn daarmee enkel kwantitatief. Hoewel in dit proefschrift het DEB model niet in alle volledigheid terugkomt, speelt de DEB filosofie wel een sleutelrol. In het bijzonder komt het idee terug om traditioneel volledig gescheiden soorten te combineren in één model: fytoplankton dat energie betrekt van zonlicht en bacteriën die energie betrekken van organisch materiaal worden verenigd in een mixotroof, die zowel zonlicht als organisch materiaal kan benutten. Een dergelijke combinatie van strategieën komt veel voor in plankton. Daarnaast komt een scala aan DEB elementen terug in de diverse modellen in dit proefschrift. Deze elementen omvatten onder andere de manier om de afhankelijkheid van meerdere substraten te modelleren en om compromissen ("trade-offs") te formuleren als de verdeling van een beperkte hoeveelheid energie over verschillende activiteiten, bv. het opvangen van licht en het opnemen van nutriënten.

**Ingrediënten**

De belangrijkste premisse in dit proefschrift is dat een realistisch ecosystems kan zelforganiseren uit een groot aantal willekeurig gekozen soorten, die onderling de
competitie aangaan. Dit idee is recentelijk onafhankelijk ontwikkeld en toegepast op planktongemeenschappen, maar met een "botte bijl"methode waarbij allerlei verschillend gemodelleerde soorten concurreren in een model van de wereldzeeën. Dit leidde weliswaar tot interessante resultaten, maar vereist enorme rekenkracht. Daardoor kan het model maar door weinigen worden gebruikt, en leent het zich nauwelijks voor experimenten waarvoor herhaaldelijke modellsimulaties nodig zijn.

In dit proefschrift worden alle soorten gemodelleerd met hetzelfde, universele model. Ze variëren enkel in de waarde van een beperkt aantal eigenschappen, vertegenwoordigd door modelparameters. Door deze constructie wordt de soortsamenstelling van het systeem volledig samengevat door de frequentieverdeling van de waarden van geselecteerde soorteigenschappen. Deze verdeling kan expliciet gemodelleerd worden door voor iedere eigenschap een groot aantal mogelijke waarden te kiezen, en dan voor iedere combinatie van eigenschappen een aparte soort in het systeem te plaatsen. Dat gebeurt bijvoorbeeld in hoofdstuk 2, waarin een totaal van 625 virtuele soorten meegenomen wordt. Dit levert een realistisch ecosysteem op, dat zelforganiseert vanuit een beperkt aantal simpele regels, maar het vereist veel rekenkracht.

Doordat alle soorten kwalitatief identiek zijn, wordt het wiskundig mogelijk om de frequentieverdeling van eigenschappen samen te vatten met de totale biomassa in het systeem, de gemiddelde eigenschappen van alle soorten, en de variatie in eigenschappen (een maat voor biodiversiteit). Hoofdstuk 3 laat zien dat de verandering van deze samenvattende statistieken kan worden afgeleid vanuit het gedrag van individuele soorten. Belangrijk is dat deze samenvattende beschrijving op zichzelf staat: de verandering in totale biomassa en in het gemiddelde en de variatie van eigenschappen kan worden beschreven zonder dat de individuele soorten terugkomen in het model. Hierdoor wordt het model veel simpeler: met minder dan tien variabelen kunnen de belangrijkste aspecten van de soortsamenstelling van het ecosysteem worden beschreven. Het resulterende model vereist weinig rekenkracht en is daarom bij uitstek geschikt voor toepassing in ruimtelijk gestructureerde modellen, waarin honderdduizenden ruimtelijk gescheiden ecosystemen worden gemodelleerd, en voor parameterschatting waarbij tienduizenden simulaties nodig zijn om de parameterwaarden te vinden die het best passen bij observaties.

Ruimte en tijd

In een constante omgeving kunnen meerdere concurrerende soorten maar zelden naast elkaar bestaan: meestal verdringt één soort alle anderen. Dit fenomeen wordt competitieve exclusie genoemd door modellers. Tot op zekere hoogte kan dit beschouwd worden als een modeleigenaardigheid: doordat interacties tussen soorten in modellen niet of versimpeld worden meegenomen is co-existentie niet mogelijk. Toch is waarschijnlijk dat een constante omgeving ook in werkelijkheid veel minder diversiteit toestaat dan een variabele omgeving: seizoens- en ruimtelijke variatie in factoren zoals licht en temperatuur spelen waarschijnlijk een belangrijke rol bij de
handhaving van biodiversiteit. Bij het testen van modellen waarin de soortenbeschikking expliciet wordt meegenomen is het daarom van belang om ook de variabiliteit van de omgeving te beschrijven.

Voor plankton spelen vooral variatie in diepte en tijd een belangrijke rol. Plankton bevindt zich over het algemeen in de bovenste 75-150 m van de oceaan. Dat is minder dan 5% van de gemiddelde diepte van de oceaan, maar over deze relatief korte afstand treden al enorme variaties op: de lichtintensiteit neemt af met een factor 100, de temperatuur daalt met 10°C of meer, en de nutriëntconcentraties stijgen met soms wel een factor 100. Om dergelijke variaties te meemaken wordt de omgeving van het plankton in hoofdstuk 1 en 3 gemodelleerd als een waterkolom, waarbij de afstand van oppervlak tot zeebodem wordt onderverdeeld in honderd lagen, ieder met een eigen lokale planktongemeenschap. Deze lagen staan natuurlijk niet los van elkaar: diffusie zorgt dat er uitwisseling tussen naburige lagen optreedt. Onder invloed van koude en wind aan de oppervlakte kan door turbulentie de uitwisseling tussen lagen nog veel sterker worden. Zulke turbulent menging treedt vooral op in de herfst en winter, en is dan zo hevig dat het grote consequenties heeft voor het ecosysteem: algen worden van het oppervlak getransporteerd naar de donkere diepe, en nutriënten worden aan het oppervlak gebracht. Dit heeft drastische gevolgen: het systeem wordt teruggezet naar een situatie met nagenoeg geen biomassa en veel nutriënten. Om deze belangrijke rol van turbulentie mee te nemen in het model wordt gebruik gemaakt van het General Ocean Turbulence Model (GOTM), wat gespecialiseerd is in het berekenen van de intensiteit van turbulent menging. Om de seizoensinvloeden op turbulentie, licht en temperatuur nauwkeurig te beschrijven worden de waterkolom aan het oppervlak blootgesteld aan waargenomen weersomstandigheden. Hierdoor worden zowel de seizoenspatronen in licht en temperatuur meegenomen, als ook onvoorspelbare dag-tot-dag variatie.

Toepassing op plankton
Door echte weersomstandigheden mee te nemen en de verschillende waterlagen expliciet te beschrijven, wordt het mogelijk om in detail te kijken naar de variatie in de soortenbeschikking van planktongemeenschappen in diepte en tijd. Dit wordt gedaan in hoofdstuk 2 en 4.

Hoofdstuk 2 test de klassieke hypothese die stelt dat veranderingen in de soortenbeschikking van plankton bepaald worden door competitie voor licht en nutriënten. Het kijkt daarvoor naar het gedrag van een simpele fytoplanktongemeenschap. Verschillen tussen soorten worden aangebracht in de mate waarin ze investeren in het actief benutten van licht en nutriënten. Hierbij zijn soorten met een hoge investering in het voordeel tijdens perioden van schaarste, en in het nadeel (omdat ze overdreven veel investeren) in tijden van overvloed. Dit model reproduceert twee belangrijke patronen. Ten eerste ontstaat in diepere waterlagen een gemeenschap die veel energie steekt in het opvangen van licht. Dit komt in werkelijkheid overeen met een hoge productie van chlorofyl: het pigment waarmee
licht wordt opgevangen. Dergelijke gemeenschappen worden in de natuur onderdaad waargenomen in dieper water. Ten tweede is er een verschuiving zichtbaar van soorten met lage investering in nutriëntacquisitie in de lente (wanneer wintermenging veel nutriënten aan het oppervlak heeft gebracht) naar een hoge investering in de zomer (wanneer nutriënten schaars geworden zijn). Dit komt goed overeen met klassieke theorie.

Hoofdstuk 4 breidt de planktongemeenschap uit met de mogelijkheid om organisch materiaal te gebruiken als energiebron. Hierdoor omvat het model niet alleen fytoplankton, maar ook bacteriën. Daarnaast kan het omgaan met fytoplanktonsoorten die naast licht ook in staat zijn om organisch materiaal te gebruiken; dergelijke "mixotrofen" wordt steeds vaker waargenomen. Soorten worden nu onderscheiden op basis van hun investering in de benutting van licht (autotrofie) en organisch materiaal (heterotrofie). Dit model reproduceert een verbazend aantal natuurlijke patronen, waaronder de verschuiving van autotrofie via mixotrofie naar heterotrofie van lente tot herfst, de vorming van een diepe gemeenschap van autotrofen die rijk zijn aan chlorofyl, en een piek in biodiversiteit in de lente. Dit maakt het aannemelijk dat de verschillen in soortsamenstelling in plankton beter kunnen worden toegeschreven aan competitie voor verschillende energiebronnen, dan aan competitie voor nutriënten.

Identificatie van belangrijkste eigenschappen

Hoofdstuk 5 introduceert een manier om met beperkte informatie toch een idee te krijgen van de waarschijnlijke eigenschappen van iedere willekeurige soort. Deze methode maakt gebruik van informatie over de evolutie van soorten: als twee soorten evolutionair (genetisch) nauw verwant zijn, is het aannemelijk dat hun eigenschappen vergelijkbaar zijn. Om een eigenschap van een gegeven soort te reconstrueren worden alle observaties daarom gewogen naar de hun verwantschap met die soort. Dit blijkt een zeer effectieve manier om tot de best mogelijke schattingen te komen voor soorteigenschappen. Dit wordt verder geïllustreerd in hoofdstuk 6, waarin de methode wordt toegepast op een grote, nieuw aangelegde collectie met observaties van eigenschappen van fytoplankton in zoetwater. Het blijkt dat veel van deze eigenschappen erfelijk zijn, en dat de methode gebaseerd op
verwantschap dus zeer zinnig is. Daarnaast blijkt dat de verschillen tussen soorten bijzonder goed worden samengevat door een enkele, basale eigenschap: de celgrootte. Deze heeft voorspellende waarde voor veel andere eigenschappen, waaronder de groeisnelheid (grote soorten groeien langzamer) en predatiegevoeligheid (kleine soorten worden meer gegeten). Dit zijn belangrijke gegevens voor toekomstige planktonmodellen.

Toekomst

De waarde van dit proefschrift ligt in de eerste plaats in de introductie van een volledig raamwerk voor het modelleren van ecosystemen op basis van (1) een universeel model voor alle soorten, (2) kwantitatieve verschillen in soorteigenschappen, en (3) zelforganisatie van het ecosysteem door competitie. Dit raamwerk wordt gedemonstreerd met kwalitatieve vergelijkingen met natuurlijke planktongemeenschappen. De lezer zou dan ook achter kunnen blijven met de vraag of dergelijke modellen wel gebruikt kunnen worden voor het doen van gedetailleerde kwantitatieve voorspellingen, zoals nodig voor het bestuderen van de organische koolstofpomp. Het antwoord op deze vraag is volmondig "ja". Tijdens dit onderzoek zijn er diverse studies afgesplitst die zich richten op kwantitatieve vergelijkingen met observaties. Deze zijn nog niet volledig afgerond, en ontbreken daarom in dit proefschrift. Ter afsluiting noem ik daarom nog enkele van de voorlopige resultaten.

Het mixotrofe model uit hoofdstuk 4 is uitgebreid gekalibreerd tegen duizenden observaties nabij Bermuda, en blijkt de patronen in nutriënten, chlorofyl, primaire productie en het zinken van organisch materiaal in diepte en tijd goed te reproduceren. Het model is vervolgens opgenomen in een volledige beschrijving van de wereldzeeën, en blijkt goed opnieuw goed in staat om (kwantitatief) biomassa, primaire productie en (kwalitatief) biodiversiteit te voorspellen - over de hele wereld, ondanks het feit dat het model enkel voor Bermuda geoptimaliseerd is! In recente vergelijkingen tussen resultaten van tientallen planktonmodellen op wereldschaal komt het mixotrofe model er dan ook goed uit (in de top 3), terwijl het model in verhouding bijzonder simpel is (beter presterende modellen bevatten meer dan 10 keer zoveel variabelen en parameters). Als laatste zijn de resultaten van de analyse uit hoofdstuk 6 gebruikt om een minimaal fytoplankton-zoöplankton model te formuleren voor een groot meer, de Bodensee, met de grootte van fytoplankton als enige eigenschap. Dit model reproduceert zowel de biomassa van fytoplankton en zooplankton, als ook het gemiddelde en de spreiding van de celgrootte van fytoplankton door het jaar heen. De reproductie van de spreiding in celgrootte is uitzonderlijk – het suggereert dat dit type model zelfs kwantitatieve voorspellingen kan produceren voor de biodiversiteit in natuurlijke systemen.

Met de kwalitatieve en kwantitatieve validatie van het nieuwe raamwerk achter de rug begint in zekere zin het echte werk pas: de methode kan ingezet worden om gericht vragen te beantwoorden over de relatie tussen de soortsamenstelling en het functioneren van natuurlijke systemen. Een eerste voor de hand liggend onderwerp is
de relatie tussen planktongemeenschappen en stofstromen (koolstof, maar ook stikstof, fosfor en silicium), waarbij zeker is dat de soortsamenstelling van het plankton een cruciale rol speelt. Dit is het onderwerp waarin ik in de komende jaren verder aan zal werken. Hier hoeft het echter niet bij te blijven: de methode beschrijft het functioneren van ecosystemen in de meest algemene zin, en kan daarmee overal in de ecologie worden gebruikt. Het aantal potentiële toepassingen is daarmee vrijwel onbeperkt.
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